SETTING PRIORITIES FOR AMBIENT AIR QUALITY OBJECTIVES

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SETTING PRIORITIES

FOR

AMBIENT AIR QUALITY OBJECTIVES

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FOREWORD

Alberta Environment, with the assistance of the Clean Air Strategic Alliance, held a multi-stakeholder workshop in October 2000 to set priorities for Alberta's Ambient Air Quality Objectives. A three-year work plan ending March 31, 2004 was developed from the workshop recommendations.

In order to develop a new three-year work plan, a multi-stakeholder workshop was held in October 2004. This study was commissioned in preparation for the workshop to provide background information on alternative, science based, and cost effective methods for setting priorities.

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GLOSSARY

ARET	Accelerated Reduction/Elimination of Toxics
BEES	Building for Environmental and Economic Sustainability
BUA	Beratergremium für Altstoffe (German Chemical Society Advisory Committee on Existing Chemicals)
CAP	Criteria Air Pollutants
CCME	Canadian Council of Ministers of the Environment
CEPA	Canadian Environmental Protection Act
CESARS	Chemical Evaluation Search and Retrieval System
CML	Centrum voor Milieuwetenschappen Leiden (Leiden University Institute of Environmental Sciences)
DALY	Disability Adjusted Life Years
EPA	Environmental Protection Agency
EURAM	European Union Risk Ranking Method
FDA	Food and Drug Administration
HAP	Hazardous Air Pollutants
HPVC	High Production Volume Chemical
IUCLID	International Uniform Chemical Database
LCA	Life Cycle Assessment
LPVC	Low Production Volume Chemical
NERAM	Network for Environmental Risk Assessment and Management
NFPRER	National Framework for Petroleum Refinery Emission Reductions
NIST	National Institute of Standards and Technology
NPRI	National Pollutant Release Inventory
OECD	Organization for Economic Co-operation and Development
OPPT	Office of Pollution Prevention and Toxics
PBT	Persistent, Bioaccumulative and Toxic
QSAR	Quantitative Structure Activity Relationship
RSEI	Risk Screening Environmental Indicators
SETAC	Society of Environmental Chemistry and Toxicology
SMILES	Simplified Molecular Input Line Entry System
TRACI	Tool for the Reduction and Assessment of Chemical and other environmental Impacts
USDA	United States Department of Agriculture
VOC	Volatile Organic Compound

SUMMARY

The goals of this study were to review, analyze and assess successful priority setting techniques used by other jurisdictions; and use these results to develop a recommended approach for setting ambient air quality objective priorities that integrates the concerns of stakeholders with Alberta Environment requirements.

To fulfil these objectives, existing priority-setting techniques used by other jurisdictions were identified and documented through a literature and expert review. A review of published literature for descriptions of priority setting methodologies was conducted. This process identified twelve priority setting methodologies or tools relevant to the study goals.

Based on the results of the literature and expert review, several techniques were identified for further investigation through interviews. Practitioners were identified and agreed to be interviewed or answer questions concerning four methods. The purpose of the interviews was to gain more insight into the practical use of the prioritization process, its strengths and weaknesses, and how it is, or might be, applied in a multi-stakeholder setting.

An analysis process was developed to identify the strengths and weaknesses of each methodology or tool, and assess its suitability for use in setting priorities for ambient air quality objectives. A well-known framework for chemical screening approaches was used as a starting point for further analysis and assessment. Each technique was also assessed for its ability to take into account the complete pathway (i.e. release, transport/fate, exposure, effect) between chemical emissions and damage to human health or the environment. The key strengths and weaknesses of each technique (overall and in terms of their usefulness for setting priorities for ambient air quality objectives) were identified.

Based on the analysis, it appears that TRACI is the most promising technique, because 1) it considers the complete pathway (i.e. release, fate, exposure, effect) between chemical emissions and damage to human health or the environment; 2) it considers both human health and ecosystem effects (i.e. damages); and 3) it does not appear to be too resource intensive (i.e. time and effort) to use.

Some considerations for using TRACI to help set priorities for ambient air quality objectives are presented. One of the key challenges will be to ensure that a comprehensive and accurate inventory of Alberta air emissions is available to use with the TRACI methodology. The most relevant TRACI impact categories to use include three varieties of Human Health (Cancer, Non-Cancer and Criteria), Ecotoxicity and Photochemical Smog. If desired, a single score for each chemical could be derived – this would involve some additional effort to normalize impact scores. If a single score approach is not used, then priorities could be derived for each individual impact, and an overall priority list developed using a combination of analysis of the individual impact priority lists, expert judgement and stakeholder input.

1.0 INTRODUCTION

Alberta currently has ambient air quality objectives in place for several substances including six common air pollutants (also known as "criteria air contaminants"), 28 air toxic substances (also known as "hazardous or toxic air pollutants") and five "other" air quality parameters.[1] A regular process is in place to determine if additional air quality objectives are required or if existing objectives should be changed. This process requires a priority setting methodology to identify the highest priority substances that may require an ambient air quality objective to protect ecosystems and public health. The methodology should be rigorous, transparent and cost effective.

The goals of this study were to review, analyze and assess successful priority setting techniques used by other jurisdictions; and use these results to develop a recommended approach for setting ambient air quality objective priorities that integrates the concerns of stakeholders with Alberta Environment requirements.

Based on experience with the last priority setting process for ambient air quality objectives that occurred in October 2000, the "new" priority setting methodology should meet the following objectives:

- It should be based solidly on science;
- It should be transparent;
- It should be repeatable;
- It should take into account stakeholder concerns; and
- It should be cost effective.

1.1 Scope of Decisions Supported

It is important to understand the overall process for setting ambient air quality objectives and how priority setting fits into that overall process. Of particular interest is the scope of decisions that will be supported by the recommended priority setting methodology. The overall process and decisions supported are described in the document "Alberta Ambient Air Quality Guidelines Work Plan" (Alberta Environment (2001)).[2] The following information is taken from that document.

> There are four processes for ambient air quality objective development (see Table 1). The process to be followed depends on whether an objective already exists in Alberta, and whether the substance or objective in question is a stakeholder priority or has been identified as a "department need". Department needs arise from various sources,

[1] See Appendix 1 for a list of these and http://www3.gov.ab.ca/env/protenf/standards/index.html for details
[2] Available at http://www3.gov.ab.ca/env/protenf/publications/AlbertaAmbientAirQualityGuidelinesWorkPlan.pdf

including but not limited to provincial regulations and proposals for new industrial facilities.

Table 1 Development processes for Ambient Air Quality Objectives

	No Existing Objective	Existing Objective
Stakeholder Priority	Create	Review
Alberta Environment Need	Adopt	Update

The decision to **create** a new ambient air quality objective is considered when there is no existing objective in place, and the substance has been identified as a stakeholder priority.

The decision to **review** an existing ambient air quality objective is considered when there is an existing objective in place, and that objective has been identified as a stakeholder priority.

The decision to **adopt** a new ambient air quality objective (from another jurisdiction) is considered when there is no existing objective in place, and the substance has been identified as an Alberta Environment need.

The decision to **update** an existing ambient air quality objective is considered when there is an existing objective in place, and Alberta Environment needs that objective to be updated.

Source. Adapted from Alberta Environment (2001): Alberta Ambient Air Quality Guidelines Work Plan

In addition to the factors discussed above, other considerations such as time and resource constraints are important in determining the amount of time and effort available to create, review, adopt or update ambient air quality objectives. Since there is likely to always be a higher demand for ambient air quality objectives than time and resources available to meet that demand, it is important to set priorities so that the most important needs are addressed first.

1.2 Limitations and Assumptions

Time and resource constraints limited the scope of this study, in particular the review of existing priority setting methodologies. The potential scope for such a review is almost unlimited. The methodologies that were reviewed represent a range of approaches, range of prioritization functions and balance between North American and European methods.

It is important to keep in mind that the scope of this study was priority setting only. Hence the rigor associated with risk assessment is not applicable or feasible, given the scale and scope of

priority setting for ambient air quality objectives. In most cases, the methods reviewed are not appropriate for detailed, site-specific risk assessment.

A peer/expert review process has not been conducted on this study.

For the purposes of this study, priority setting exists within the context of an overall development process for ambient air quality objectives. The design of this overall development process is outside the scope of this study.

The status of existing Alberta emissions inventories was not a focus of this study. However, it is clear that many of the techniques reviewed as part of this study require a comprehensive and accurate inventory of air emissions to support priority setting.

2.0 METHODOLOGY

To fulfil the objectives identified above, existing priority-setting techniques used by other jurisdictions were identified and documented through a literature and expert review, and additional information about some of these was gathered by interviewing selected practitioners. Each of these steps is discussed in more detail below.

2.1 Literature and Expert Review of Methodologies

A review of published literature for descriptions of priority setting methodologies was conducted. Sources of information consulted included expert opinions, printed materials, electronic documents available on the Internet, and journal articles. Although the focus of this study was ambient air quality management, the scope of the literature and expert review included other environmental releases and media, since methodologies from other environmental disciplines could be transferable and applicable to ambient air quality management, and there was very little information available about methodologies or tools that directly applied to ambient air quality management.

This process identified twelve priority setting methodologies or tools that met the following criteria:

- Written descriptions were available and transparent;
- Methodology was rigorous and science based;
- Either directly or indirectly applicable to ambient air quality, or offered insights into the priority setting process;
- Covered a range of prioritization functions (see Table 2);
- Covered a range of approaches towards setting priorities; and
- Balanced between North American and European sources.

The methodologies and tools identified covered a range of functions that could be used in a priority setting process. The widest range of generic "prioritization functions" in the literature reviewed was described by Environment Canada (1994a), and is shown in Table 2. This list of functions was used as a general framework for categorizing the methodologies and tools identified. Note that these functions are not always applied in a linear fashion (i.e. step 1, step 2, step 3, etc.). Some priority setting methods may use an iterative process. For example, the *characterize* function may be used more than once in the overall priority setting process.

Table 2 Generic prioritization functions

Function	Description
Scan & Scope	Identify and describe the full universe of items that need to be prioritized
Screen	Apply criteria to eliminate some items and identify the most significant items
Characterize	Measure or estimate the quantitative value of parameters for various items (note: this function can be used to support *screening* or *scoring*)
Score	Score the various items according to their impacts on human health, ecosystems, etc.
Rank & Cluster	Group the items into clusters (e.g. high, medium, low priority) to determine next steps (e.g. manage, research, monitor)

Source: Adapted from Environment Canada (1994a).

The twelve priority setting methodologies or tools identified are summarized in Table 3, and a more detailed profile for each is included in Appendix 2. Each profile includes the following information:

- Prioritization functions that the method includes (see Table 2);
- Description of the methodology or tool;
- Data requirements;
- Sources of data;
- Outcomes;
- Resources required to use the methodology or tool;
- Constraints; and
- Examples of use (if applicable).

As shown in Table 3, some of the methods cover only a few of the generic prioritization functions, and others cover all of them. Many of the techniques come from the field of chemical prioritization (i.e. chemical ranking and scoring), while some have been applied to environmental issue prioritization or are applied more broadly for processes such as selection of new technologies.

Based on the results of the literature and expert review, several techniques were identified for further investigation through interviews.

Table 3 Priority setting methodologies and tools reviewed

Methodology or Tool	Origin	Scope	Prioritization Functions
ARET Substance Selection Process	Environment Canada and ARET stakeholders	Identify prioritized list of toxic substances using PBT screens for action under ARET	Screen Characterize Score
ChemSTEER	U.S. EPA	Estimate occupational exposure to substance Estimate releases of substance from industry	Characterize
Endocrine Disruptor Screening Program	U.S. EPA	Screening of potential endocrine disrupters to identify priority substances for further testing	Scan & Scope Screen
Environmental Issue Definition and Ranking	Environment Canada	Identify highest priority environmental issues for management through various options	Scan & Scope Screen Characterize Score Rank & Cluster
EURAM: EU Existing Chemicals Regulations	European Union	Identify high risk chemicals for priority substance lists and priority chemicals for further assessment	Scan & Scope Screen Characterize Score Rank & Cluster
German Existing Chemicals	German Chemical Society	Identify priority chemicals for further detailed assessment	Scan & Scope Screen Characterize Score Rank & Cluster
HEIDI: Health Effects Indicator Decision Index	CCME/NERAM	Ranking of releases from oil refineries by regional health effects, to set emission reduction priorities	Characterize
Intake Fraction Analysis	U.S.	Estimate fraction of chemical released that eventually passes to human population	Characterize
Multiple Issue Contribution Analysis	Various	Weighting and scoring of different environmental impacts according to value judgements	Score Rank & Cluster
PBT Profiler	U.S EPA, Chemical Industry and Environmental Defense NGO	Screen chemicals for persistence, bioaccumulation and toxicity	Screen Characterize
Risk Screening Environmental Indicators	U.S. EPA	Provides release, hazard and risk based indicators for all U.S. TRI chemicals	Screen Characterize
TRACI. Tool for the Reduction and Assessment of Chemical and other environmental Impacts	U.S. EPA	Assessment of potential chemical impact in 12 environmental impact categories	Characterize

2.2 Interviews with Selected Jurisdictions

Practitioners were identified and agreed to be interviewed or answer questions concerning the following methods:

- Endocrine Disruptor Screening Program
- EURAM: EU Existing Chemicals Regulations
- German Existing Chemicals
- Multiple Issue Contribution Analysis

The purpose of the interviews was to gain more insight into the practical use of the prioritization process, its strengths and weaknesses, and how it is, or might be, applied in a multi-stakeholder setting. The people interviewed were practitioners in various jurisdictions that have experience applying the prioritization technique in question. Some of the practitioners were not available for an interview and instead provided written answers to the interview questions.

To the extent possible, the interview results that apply directly to the specific methodology or tool were incorporated into the profiles shown in Appendix 2. Some additional general insights about the priority setting process were also gained from these interviews and are shown below.

- Setting priorities takes a long time: the time and effort involved is typically much higher than originally estimated;
- Rigour is appropriate, but should be matched to the overall goal (in this case, identifying a high priority list of substances, not risk assessment);
- Decisions should be based on needs (i.e. priorities must address environmental stressors);
- A relative ranking of substances is required, not an absolute scoring of each;
- A priority setting methodology must be feasible and practical for a wide range of substances;
- In many cases, the data required to use a methodology or tool is not available for a broad range of substances. Hence it is important to consider ways of handling data deficiencies carefully, such as default values or considering exposure instead of hazard;
- There is always some degree of subjectivity involved, either implicit or explicit;
- It is important to recognize stakeholder limitations and to design their role appropriately e.g. members of the public might be asked to comment on which impacts are most important to them, rather than on detailed scientific data; and
- To ensure both validity and acceptance of the methodology, it is good to involve a variety of stakeholders in the process at various times.

3.0 ANALYSIS

An analysis process was developed to identify the strengths and weaknesses of each methodology or tool, and assess its suitability for use in setting priorities for ambient air quality objectives.

Pennington and Bare (2001) presented the hierarchical framework of chemical screening approaches shown in Table 4, based on the degree of representation and level of sophistication used to model chemical fate, exposure and human health/environmental effects. Although this model does not apply to all the methodologies and tools identified and reviewed, it provides a useful framework and starting point for further analysis and assessment.

Table 4 Hierarchical framework of chemical screening approaches

Complexity & Data Needs	Group	Description	Fate and Exposure Measures	Effect Measure
Low	1	Direct summation of emissions data	None	None
	2	Comparison in terms of effect	None	Selected toxicological measures and/or benchmarks
	3	Scoring and ranking	Selected parameters such as degradation half-life and bioaccumulation measures	Selected toxicological measures and/or benchmarks
	4	Model-based approaches	Integrated model predictions of fate and exposure (intake fractions)	Selected toxicological benchmarks and/or dose-response measures
High	5	Site-specific risk assessment	Site-specific fate and exposure estimations using models and/or measurements	Generic or site-specific toxicological benchmarks and/or dose-response measures

Source Pennington and Bare (2001), adapted from Pennington and Yue (2001)

Group 1 approaches simply look at mass of emissions to identify the substances with the highest emissions on a mass basis. This approach is often used by regulatory agencies when presenting the results of emissions inventories such as the National Pollutant Release Inventory (NPRI). It has the advantage of simplicity, but does not take into account the relative harm caused by various substances, where they are released, what happens to them, what populations or ecosystems are exposed to them and how these populations or ecosystems are affected.

Groups 2 through 5 approaches are increasingly more sophisticated through additional consideration of chemical fate, exposure and effect, as shown in Table 4.

The more complex and sophisticated approaches are more representative of reality and, if applied properly, could result in a better ranking of priority substances. However, it is also important to note that the more detailed site-specific approaches are less applicable to a large region such as Alberta. Pennington and Bare (2001) point out that the suitability of a given group of approaches for a particular application depends on a number of factors, including:

- The relative environmental behaviour of the chemicals considered;
- The quality of available data;
- The comprehensiveness of the model; and
- The ability of more resource-intensive techniques to actually provide an improvement in discrimination [between chemicals].

Where appropriate, the methodologies or tools reviewed were classified according to the hierarchical framework shown in Table 4. Each technique was also assessed for its ability to take into account the complete pathway (i.e. release, transport/fate, exposure, effect) between chemical emissions and damage to human health or the environment:

The key strengths and weaknesses of each technique (overall and in terms of their usefulness for setting priorities for ambient air quality objectives) were identified and are shown in Table 5. More detail about the weaknesses for each methodology or tool is shown under "Constraints" in the detailed profiles in Appendix 2.

Based on the analysis shown above in Table 5, it appears that TRACI is the most promising technique, considering the following criteria:

- It considers the complete pathway (i.e. release, fate, exposure, effect) between chemical emissions and damage to human health or the environment;
- It considers both human health and ecosystem effects (i.e. damages); and
- It does not appear to be too resource intensive (i.e. time and effort) to use.

TRACI uses the concept of impact categories to consider a range of potential environmental impacts. It uses 12 impact categories, some of which are shown in Table 6. Not all of these are applicable to ambient air quality – Table 6 indicates those that are. These include:

- Human Health Cancer
- Human Health Non-Cancer
- Human Health Criteria (Human health impacts from criteria air contaminants)
- Ecotoxicity
- Photochemical Smog

Table 5 Strengths and weaknesses of methodologies reviewed

Methodology or Tool	Release	Fate	Exposure	Effect	Group	Strengths	Weaknesses
ARET Substance Selection Process		√		√	3	Provides scoring and cut-off criteria Based on measured data ("worst-case") in CESARS database	Focuses on intrinsic properties of chemical Doesn't consider actual releases, exposures, or damages
ChemSTEER	√	√	√		4	Easy access to a range of models Fast screening of new and existing chemicals	Workplace health focus Not applicable to most chemicals that are gases in ambient conditions
Endocrine Disruptor Screening Program		√	√	√	2	Identifies priority substances for further assessment	Endocrine disruption effects only Lack of data on endocrine disrupting effects Limited to pesticide residues on 20 most consumed food items
Environmental Issue Definition and Ranking		√	√	√	n/a	Comprehensive process for priority setting	Focus on overall environmental issues Requires substantial time and effort
EURAM: EU Existing Chemicals Regulations	√	√	√	√	4	Ranking of chemicals based on huge amount of data	Focuses on aquatic toxicity Clustering of results, related to defaults Huge effort
German Existing Chemicals	√	√	√	√	3	Sorts large number of chemicals into categories for further action	Resource intensive Not applicable to all chemicals (see profile for details)
HEIDI: Health Effects Indicator Decision Index	√	√	√	√	4	Site specific ranking of emission reductions based on health effects	Human health effects only Assumes site specific releases and population densities Resource intensive
Intake Fraction Analysis	√	√	√		3	Summarizes large amount of information about chemicals in single number	Human health only Considers only fate and exposure, not effect
Multiple Issue Contribution Analysis					n/a	Allows transparent and systematic use of value judgements to weight and score different environmental impacts Allows stakeholder input	Inherently subjective Need to clearly identify source of weighting or valuation between impacts
PBT Profiler		√		√	3	Fast early level screening of chemicals	Considers only intrinsic properties of substance Limited range of chemicals can be assessed (see profile for details)
RSEI: Risk Screening Environmental Indicators	√	√	√	√	4	Ranking of chemicals by releases, hazard or risk	Human health effects only U.S. geography specific Toxicity benchmarks incorporate policy driven safety factors No consideration of background ambient levels
TRACI	√	√	√	√	4	Characterization of chemical's potential impacts in 12 environmental impact categories	U.S. specific Potential impact only, not actual risk

Table 6 Application of Impact Categories to Ambient Air Quality

Impact Category	Description	Applicable to Ambient Air Quality? (CAP or HAP)	Available Databases and Scope	Reference unit	Comment
Acidification	A measure of emissions to air known to contribute to atmospheric acid deposition (acid rain).	No	CML[3]	kg SO_2 equivalent	
			TRACI	moles H+ equivalent	location specific characterization factors available
Global Warming (Climate Change)	A measure of greenhouse gas emissions, such as CO2 and methane. These emissions are causing an increase in the absorption of radiation emitted by the earth, magnifying the natural greenhouse effect.	No	CML	kg CO_2 equivalent	
			TRACI	kg CO_2 equivalent	
Human Toxicity	A measure of the potential toxicity to humans of substances based on the chemical condition, original emission place and fate after entering the environment. The calculation begins with emission quantities and calculates the concentrations in the environment using a distribution model. Toxicological threshold values are used, which are based on continuous exposure.	Yes	CML	kg di-chlorobenzene equivalent	
Human Health Cancer	Potential of a chemical released into an evaluative environment to cause human cancer effects.	Yes	TRACI	lbs benzene equivalent	uses CalTOX
Human Health Non-cancer	Potential of a chemical released into an evaluative environment to cause human non-cancer effects.	Yes	TRACI	lbs toluene equivalent	uses CalTOX
Human Health Criteria	Potential of a criteria air contaminant released into an evaluative environment to cause human health effects. Criteria air contaminants are solid and liquid particles commonly found in the air. They include coarse particles known to aggravate respiratory conditions such as asthma, and fine particles that can lead to more serious respiratory symptoms and disease.	Yes	TRACI	total DALYs (Disability Adjusted Life Years)	-location specific characterization factors available -uses intake fractions

[3] Centrum voor Milieuwetenschappen Leiden (Leiden University Institute of Environmental Sciences)

Impact Category	Description	Applicable to Ambient Air Quality? (CAP or HAP)	Available Databases and Scope	Reference unit	Comment
Ecotoxicity	A measure of the potential toxicity to plants, animals and other biota in the natural environment of substances based on the chemical condition, original emission place and fate after entering the environment. The calculation begins with emission quantities and calculates the concentrations in the environment using a distribution model. Toxicological threshold values are used, which are based on continuous exposure.	Yes	CML (terrestrial and aquatic)	kg di-chlorobenzene equivalent	
			TRACI	lbs 2,4-D equivalent	
Photochemical Smog	A measure of emissions of precursors that contribute to low level smog, produced by the reaction of nitrogen oxides and VOC's under the influence of sunlight Smog has a direct effect on human health, increasing the incidence of asthma It also damages plants by reducing their ability to photosynthesize.	Yes	CML	kg ethene equivalent	
			TRACI	kg NO_x equivalent	location specific characterization factors available
Eutrophication	A measure of nutrient emissions to water that can lead to increases in biomass production. In water this can lead to algal blooms resulting in oxygen depletion that affects higher species such as fish. Undesirable shifts in numbers of species can also occur resulting in a threat to biodiversity.	No	CML	kg phosphate equivalent	location specific characterization factors available
			TRACI	kg nitrogen equivalent	
Ozone depletion	A measure of emissions to air based on contribution to increase ultraviolet radiation reaching earth's surface through depletion of stratospheric ozone.	No	CML	kg CFC11 equivalent	
			TRACI	kg CFC11 equivalent	

Notes:

- The TRACI human toxicity and ecotoxicity impact categories include modeling of exposure. The human health criteria category includes a calculation to estimate change in exposure due to emissions. The human health cancer and non-cancer categories use the CalTOX model, which includes human exposures correlations.
- Characterization factors may not be available for all chemicals of interest. The human health criteria impact category contains five chemicals, human health cancer contains

152, human health non-cancer contains 309, photochemical smog contains 509 and ecotoxicity contains 161. Although most of these categories contain a wide range of chemicals, it is possible that a chemical released in significant quantities may not be found in the impact categories. It is important to note that exclusion from the impact category does not necessarily imply that the chemical has no impact.

4.0 CONCLUSIONS

4.1 Key Observations and Conclusions

1. None of the priority setting methodologies and tools reviewed was developed for the purpose of ambient air quality management. Most come from the general area of chemical screening and ranking. They have been used mostly to identify priority chemicals for management and/or further assessment.

2. Most of the techniques reviewed use a combination of measured data and models to estimate the environmental behaviour of substances, rather than relying only on measured data. This appears to be for the following reasons:

    a. It is difficult to find a consistent database with single values for various measured parameters; most databases give a range of data from various studies that are not consistent for different substances.
    b. Important data about hazardous chemicals is often not available. For example, a recent EPA study found that 55% of TRI chemicals had full OECD SIDS (Screening Information Data Set) testing available, and only 7% of other high production volume chemicals had full test data.[4]

3. There are literally hundreds of chemical screening and ranking approaches that have been developed for various purposes, including priority setting. For example, the OECD has web published a database of over 100 models (see Appendix 3), and an earlier study by Davis et. al. (1994b) identified 51 approaches. Available time and resources did not allow a comprehensive review of all available approaches.

4. Only one of the priority setting techniques reviewed (i.e. TRACI), considers the complete pathway (i.e. release, fate, exposure, effect) between chemical emissions and damage to human health or the environment; considers both human health and ecosystem effects (i.e. damages); and does not appear to be too resource intensive (i.e. time and effort) to use.

4.2 Using TRACI to Set Priorities

The following considerations will be useful in using TRACI to help set priorities for ambient air quality objectives in Alberta.

The TRACI model and a comprehensive inventory of air emissions in Alberta can be used to develop a first pass list of priorities for ambient air quality objectives. The following impact

[4] US EPA (1998). Chemical Hazard Availability Study Available at http.//www.epa.gov/chemrtk/hazchem.htm

categories from TRACI are relevant to ambient air quality: three varieties of Human Health (Cancer, Non-Cancer and Criteria), Ecotoxicity and Photochemical Smog. This process will result in a list of priority substances for each of the five impact categories. At this stage in the process, there are two alternatives for developing a single list of priority substances:

1. An overall priority list could be developed using a combination of analysis of the individual priority lists from each of the five impact categories, expert judgement and stakeholder input; or
2. An overall priority list could be developed using a combination of normalization and valuation as described below and in the example shown in Table 7, using the multiple issue contribution technique described in Appendix 2.

To develop an overall priority list using the multiple issue contribution technique, normalization and valuation are required. Normalization ensures that impact categories with different units of measurement are not added together. For each chemical, a relative score for each impact category can be calculated by comparing the impact score for that chemical to the impact score for all chemicals in the total inventory of Alberta air emissions. This creates a score that measures how much of the overall impact in Alberta is due to each chemical.

Valuation is required to reflect the relative importance or weighting of each of the five impact categories. There is no scientifically valid method for determining the "proper" valuation or weighting of each impact category, because this is essentially a question of values (e.g. which is more important between human health and ecosystem health?). Thus valuation becomes essentially a question of determining the values of experts, stakeholders or the general public. For more information, see the description of the multiple issue contribution technique described in Appendix 2.

The example in Table 7 shows that for impact category 1, chemical 3 contributes the most to the problem. For impact category 2, chemical 1 contributes the most to the problem. Considering both impact categories and their weighting, chemical 3 is the highest priority, followed by chemical 2, then chemical 1.

Table 8 shows how the prioritization functions identified above (see Table 2) could be implemented using the TRACI approach.

As much as possible, use the "off the shelf" TRACI characterization factors for the first round of priority setting. As experience with this technique develops, opportunities to customize this approach should be identified and implemented as time and resources permit.

Consult with Alberta air inventory specialists to ensure the most current and comprehensive inventory of air emissions in Alberta is available to use for priority setting purposes. The National Pollutant Release Inventory (NPRI) is a database of information administered by Environment Canada on annual releases to air, water, and land, and off-site transfers for disposal

Table 7 Example priority setting using multiple issue contribution

	Chemical 1	Chemical 2	Chemical 3
Impact Category 1			
Raw Score	10,000	20,000	30,000
Units	kg CO_2 equivalent		
Total Alberta Score for Impact Category 1	1,000,000		
Relative Score (A)	0.01	0 02	0.03
Weighting of Impact Category 1 (B)	20%		
Weighted Score (A x B)	0 002	0.004	0.006
Impact Category 2			
Raw Score	500	400	300
Units	kg NO_x equivalent		
Total Alberta Score for Impact Category 2	10,000		
Relative Score (C)	0.05	0.04	0.03
Weighting of Impact Category 2 (D)	10%		
Weighted Score (C x D)	0.005	0.004	0 003
Weighted Score (A x B) + (C x D)	0.007	0 008	0.009

Note. Example for illustrative purposes only

Table 8 Prioritization functions for approach using TRACI

Function	Description	Recommended Approach
Scan & Scope	Identify and describe the full universe of items that need to be prioritized	Choose inventory of air emissions
Screen	Apply criteria to eliminate some items and identify the most significant items	Select relevant TRACI impact categories for air quality objectives
Characterize	Measure or estimate the quantitative value of parameters for various items (note: this function can be used to support *screening* or *scoring*)	Apply TRACI characterization factors to air emissions inventory
Score	Score the various items according to their impacts on human health, ecosystems, etc.	Rank by individual impact category, and/or Create single score using multiple issue contribution
Rank & Cluster	Group the items into clusters (e.g. high, medium, low priority) to determine next steps (e.g. manage, research, monitor)	Identify data gaps Use time/resource constraints to determine level of effort

or recycling of several hundred specified substances. To ensure a comprehensive and accurate inventory of Alberta emissions, it will be important to include activities and sources that are not included in the NPRI. These activities and sources include, but are not limited to:

- Mining operations (including oil sands)
- Oil & gas drilling operations
- Mobile sources (e.g. cars, trucks)
- Buildings (residential)
- Agricultural activities
- Waste management (e.g. Land Fill Gas)

As a check on the above approach using TRACI, a gap analysis against ambient air quality objectives in other jurisdictions could be conducted. For example, as part of it's process for setting air quality standards, the Ontario Ministry of the Environment reviewed air quality criteria and the basis for setting them from ten agencies, including the United States Federal Government, the States of California, New York, New Jersey and Michigan, the Commonwealth of Massachusetts, the World Health Organization, The Netherlands, the Swedish Institute of Environmental Medicine and the Canadian Federal Government (CEPA).[5] For the Alberta gap analysis, it may be more appropriate to review air quality criteria and the basis for setting them from jurisdictions with similar emissions profiles, similar geography, and similar climate.

[5] Ontario MOE (2002)

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APPENDICES

APPENDIX 1: EXISTING ALBERTA AIR QUALITY OBJECTIVES[6]

Substance	Included in NPRI?
Common Air Pollutants	
1. Sulphur Dioxide	Yes
2 Hydrogen Sulphide	Yes
3 Nitrogen Dioxide	Yes
4 Carbon Monoxide	Yes
5. Ground Level Ozone	n/a (not a release)
6. Suspended Particulates	Yes
Air Toxic Substances	
1. Acetaldehyde	Yes
2. Acetic acid	No
3. Acetone	No
4. Acrylic Acid*	Yes
5 Acrylonitrile*	Yes
6 Ammonia	Yes
7. Benzene	Yes
8. Carbon disulphide	Yes
9. Chlorine	Yes
10. Chlorine dioxide	Yes
11. Chromium	Yes
12. Dimethyl ether	No
13. Ethyl chloroformate	Yes
14. Ethylene**	Yes
15. Ethlyene oxide	Yes
16. Formaldehyde	Yes
17. Hydrogen chloride	Yes ("Hydrochloric acid")
18 Hydrogen fluoride	Yes
19. Lead	Yes
20. Methanol	Yes
21. Methlyene bisphenyl diisocyanate	Yes
22. Monoethylamine	No
23. Phenol	Yes
24 Phosgene	Yes
25. Propylene Oxide*	Yes
26 Styrene	Yes
27. Sulphuric acid	Yes
28. Vinyl chloride	Yes
Other Air Quality Parameters	
1. Dustfall	
2. Coefficient of Haze	
3 Static Total Sulphation	
4. Static Hydrogen Sulphide	
5. Static Fluorides	

* Adopted January 1, 2004
**Revised January 1, 2004

[6] Source: http://www3 gov.ab.ca/env/protenf/standards/index.html

APPENDIX 2: PROFILES OF PRIORITY SETTING METHODS

ARET (Accelerated Reduction/Elimination of Toxics) Substance Selection Process

Prioritization Function

Screen
Characterization
Score

Description

The concept of ARET was developed in the early 1990's by a group of senior industry representatives and key Environmental Non-Government Organizations (ENGOs) known as the New Directions Group. In 1991 this group developed into the ARET Stakeholder committee, with the support of the federal government.

The ARET Stakeholder committee assembled a sub-committee to develop a list of priority substances for the program. The sub-committee was tasked with evaluating and prioritizing a list of over 2000 substances, using as its basis an inventory of substances found in the Great Lakes basin. Out of approximately 2000 substances in the CESARS database, about one quarter had sufficient data on toxicity, persistence and bioaccumulation to be screened for selection. Substances were scored based on available toxicity, persistence and bioaccumulation data. Scoring criteria were developed based on underlying data and cut-off scores were chosen for toxicity, persistence and bioaccumulation.

Data Requirements

The substance selection process used available data on the toxicity, persistence and bioaccumulation of the substances found in the Great Lakes basin.

Sources of Input Data

Toxicity, persistence and bioaccumulation data was obtained from the Chemical Evaluation Search and Retrieval System (CESARS). CESARS was developed by the Michigan Department of Natural Resources (MDNR), and is maintained and updated by MDNR and the Ontario Ministry of the Environment.

Outcomes

The result of this process was a list of 117 toxic substances slated for elimination or reduction. This list included 30 that persist in the environment and may accumulate in living organisms.

Resources Required

The resource requirements for this process were minimized by relying of data that was already available in CESARS. There was considerable effort needed to develop the list of substances, as it was done on a consensus basis.

Constraints

The selection of substances was limited by the lack of complete persistence, bioaccumulation and toxicity data for all the chemicals in CESARS. In this case the sub-committee chose only to consider those substances for which a complete data set was available. The prioritization was based on intrinsic properties of the substances, with no consideration of risks, emission volumes, or actual damage to the environment or to human health.

Example of Use

The ARET program ran through the 1990's, with the reduction and elimination goals set for the year 2000. The renewal of the ARET program is currently under consideration.

Sources

Environment Canada (2003). *ARET (Accelerated Reduction/Elimination of Toxics).* http://www.ec.gc.ca/nopp/aret/en/index.cfm

Environment Canada (1994b): *The ARET Substance Selection Process and Guidelines*. ARET Stakeholder Committee (Jan. 1994).

ChemSTEER: Chemical Screening Tool For Exposures & Environmental Releases

Prioritization Function

Characterization

Description

The methods in ChemSTEER were developed by the Chemical Engineering Branch of the Economics, Exposure, and Technology Division in the EPA's Office of Pollution Prevention and Toxics (OPPT). ChemSTEER allows users to select either:

- Predefined industry-specific profiles, or
- Chemical functional use-specific profiles, or
- User-defined manufacturing, processing and use operations.

EPA's OPPT uses ChemSTEER methods in screening new and existing chemicals for the potential risk they may pose to workers and the environment. ChemSTEER outputs can also be used to identify potential pollution prevention and exposure reduction opportunities.

Data Requirements

Data and information on a chemical's:

- Physical-chemical properties, including molecular weight, vapour pressure, and density.
- Production or use volume, and if applicable, fractions devoted to multiple uses.
- Weight fractions and physical states.

Case-specific parameters, when available:

- Numbers of sites, operating days, and workers; batch amounts and durations.
- Release sources and worker activities.
- Workplace concentrations and release amounts and media.
- Types and sizes of containers used to transport the chemical or mixture.

Sources of Input Data

Data on the chemical must be supplied by the user, as well as case-specific parameters. The software includes 23 models used for release and exposure assessment, as well as three industry-specific operations.

Outcomes

Using these operations and several chemical-specific and case-specific parameters and general models, the ChemSTEER computer program:

- Estimates occupational inhalation and dermal exposure to a chemical during industrial and commercial manufacturing, processing, and use operations involving the chemical.

- Estimates releases of a chemical to air, water, and land that are associated with industrial and commercial manufacturing, processing, and use of the chemical.

Resources Required

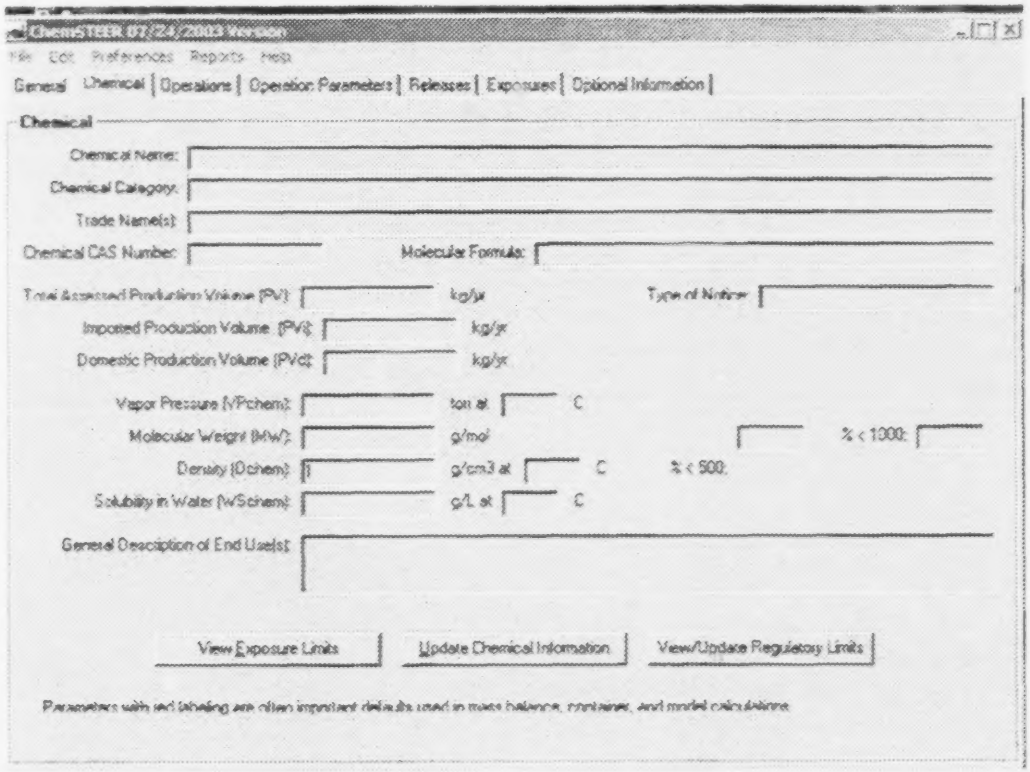
The use of this software would require a relatively minimal amount of resources, assuming easy access to the necessary chemical data.

Constraints

ChemSTEER does not contain methods for estimating exposures to chemicals to the general public, to consumers, or to other species in the environment. The software is only available as a beta version at this time. ChemSTEER is not applicable for most chemicals that are gases in ambient conditions.

Example of Use

Below is one of the data entry windows in ChemSTEER.



Sources

US EPA. Chemical Screening Tool For Exposures & Environmental Releases. 2003. http://www.epa.gov/opptintr/exposure/docs/chemsteer.htm

OECD Model Database Profile: ChemSTEER.doc

Endocrine Disruptor Screening Program

Prioritization Function

Scan and Scope
Screen

Description

The US EPA is developing a program to test an initial group of chemicals to determine whether they are endocrine disruptors. The EPA is under a congressional mandate to test all pesticides. The EPA also has discretionary authority to test non-pesticides that may have an effect cumulative to a pesticide, when a large portion of the population may be exposed to that chemical. They also have discretionary authority to test chemicals found in sources of drinking water that a substantial population is exposed to.

The Endocrine Disruptor Screening Program involves a priority setting stage, Tier 1 Screening and Tier 2 Screening. Tier 1 Screening involves a first round of basic tests to indicate whether a chemical might be an endocrine disruptor. The EPA will send any chemical that the available effects information clearly shows an endocrine-mediated effect directly to more comprehensive Tier 2 tests. Exclusions from testing include:

- Chemicals that show a very little likelihood of being endocrine modifiers (e.g. strong mineral acids, and strong mineral bases)
- Chemical mixtures (in order to gain experience with simpler single chemicals first)
- Chemicals no longer produced or used in the US

The EPA proposed an approach to establish the priority of chemicals for Tier 1 screening. The EPA wants to ensure that data-rich and data-poor chemicals were not directly compared in the priority setting process because data-poor chemicals might tend to be ranked low under such an approach. Thus, the proposed approach would establish categories of information relating to the production, release, exposure and hazard of chemicals and group the chemicals according to what data are available. This approach is termed a "compartment-based approach". The compartment-based approach is based on exposure- and effects-related compartments even though it is recognized that effects or toxicity data relevant to endocrine disruption is extremely limited for the majority of chemicals. To partly compensate for the lack of relevant toxicity data, EPA proposed to conduct a High Throughput Pre-Screening on all non-pesticide active ingredient chemicals with a production volume in excess of 10,000 pounds per year. However, it was found that this type of testing is not yet well developed enough to serve this purpose. The EPA also considered the use of Quantitative Structure Activity Relationship (QSAR) models, but found that they were not sensitive enough at this time.

It has been determined that for the initial round of Tier One testing, prioritization will be based primarily on exposure potential. Every person eats food and a significant portion of food contains some amount of pesticide residues, although usually at very low levels. Therefore, pesticide residues in food have the potential to cause widespread human exposure. Pesticides

have different use patterns and have different physical and chemical properties that affect how they move in the environment and how quickly they break down. As a result, there are often significant differences among pesticides in the proportion of food containing residues and in the levels of such residues. People also consume different amounts of different foods. All of these factors mean that people ingest greater quantities of some pesticide active ingredients than of others. To evaluate the interplay of these different variables, EPA proposes to identify the pesticide active ingredients that are most frequently found as residues on the top twenty foods that people consume. They will also take into account pesticide residues found in water, by surveying different water monitoring databases.

Data Requirements

The EPA used data on the 20 most consumed food commodities, and the pesticide residues left on those commodities, in their priority setting.

Sources of Input Data

The EPA used the most recent Continuing Survey of Food Intake by Individuals to determine the mean amount of each raw agricultural commodity consumed in the general population. The survey is part of the Food and Drug Administration's Surveillance Monitoring Program. The pesticide data is from US Department of Agriculture's Pesticide Data Program.

Having identified the top 20 foods, EPA would characterize the pesticide residue levels on these foods using information collected by two Federal agency monitoring programs, the USDA Pesticide Data Program and the Surveillance Monitoring Program conducted by FDA's Center for Food Safety and Applied Nutrition.

Outcomes

The EPA does not intend to develop an ordinal ranking of the priority chemicals that are determined through this process. They plan to designate 50 to 100 chemicals for Tier 1 Screening.

Resources Required

This process is highly resource intensive and is being carried out over a number of years. Originally the program included a database, but it was found that the time and expense to maintain it was too much, in light of the lack of data, and so existing databases are being used instead.

Constraints

This process is constrained by the lack of data on endocrine disruption. The problem of comparing data rich and data poor substances has been avoided by instead concentrating on exposure data.

Sources

US EPA. Endocrine Disruptor Screening Program, Proposed Chemical Selection Approach for Initial Round of Screening; Request for Comment. 2002. http://www.epa.gov/EPA-PEST/2002/December/Day-30/p32853.htm

Mary Belefski, U.S. EPA (Belefski.Mary@epamail.epa.gov), Personal Communication, February 2004.

Environmental Issue Definition and Ranking

Prioritization Function

Scan and Scope
Screen
Characterize
Score
Rank and Cluster

Description

This methodology has been developed by the Advisory Committee on Environmental Protection of Environment Canada, with the input of many internal and external stakeholder groups. The methodology involves four discrete steps:

1. Scan and Scope – identification and listing of all environmental problems and issues; express issues in Stress-Exposure-Response-Adaptation format; create a mini-profile sheet; test for significance; select significant issues.
2. Screen and Characterize – a checklist of criteria are applied to the issue to determine whether it is significant, whether there is jurisdiction over the issue and the information that is required to score it; the extent of the consequences are characterized.
3. Score – derive a numerical score based on ecological, health and socio-economic factors.
4. Rank and cluster – put the issues in the order determined by their scores and grouping the ranked issues (e.g. high, medium and low importance).

This methodology is part of a broader approach to decision-making, which would additionally include consultation with sectors, selection of actions and monitoring of results.

Data Requirements

For each issue, specific qualitative information is required in order to complete the scoring. For each factor, ecological, health and socio-economic, the severity, extent and trend must be scored.

Sources of Input Data

It is expected that the scoring would require the input of experts and may in some cases require further scientific research.

Outcomes

The outcome of the methodology is a ranked and clustered list of environmental issues that will feed into the next steps of the decision-making process.

Resources Required

This approach would require a considerable amount of resources, due to the expert evaluation of environmental issues. There exists the potential need for additional research in order to characterize and score the environmental issues.

Constraints

Necessary information may not always be available.

Example of Use

A Case Studies Work Book has been created which profiles a number of environmental issues, such as UVB and smog. However, this book could not be obtained.

Sources

Response Assessment Directorate, Environmental Protection Service, Environment Canada. 1994. Environmental Issue Definition and Ranking: A Proposed Priority Setting Methodology for Environment Canada.

EURAM: European Union Existing Substances Regulation

Prioritization Function

Scan and Scope
Screen
Characterize
Score
Rank and Cluster

Description

In 1993, the European Commission enacted the Existing Substances Regulation (Council Regulation (EEC) 793/93). It provided a comprehensive structure to evaluate risks posed by existing chemicals and established a procedure for treating priority lists of chemicals for immediate attention, as well as setting out the means for gathering information, requiring testing and evaluating the risks to people and the environment.

Under the regulation, evaluation and control of the risks posed by existing chemicals are carried out in four steps:

- Step 1: Data collection
- Step 2: Priority setting
- Step 3: Risk assessment
- Step 4: Risk reduction

In step one, data is collected first on High Production Volume Chemicals (HPVCs, existing chemicals imported or produced in quantities exceeding 1000 tonnes per year) and then on Low Production Volume Chemicals (LPVCs, substances in quantities between 10 and 1000 tonnes per year). Manufacturers and importers must provide production data for LPVCs, and data on production, toxicity, fate, ecotoxicity and physio-chemical properties for HPVCs.

Step two of the regulation concerns prioritizing substances that require immediate attention because of their potential effects on humans or the environment. The Commission, in consultation with the European Member States, regularly draws up lists of "priority substances". Priority substances are selected from the information submitted by manufacturers and importers to the International Uniform Chemical Database (IUCLID), and are also based on the national lists of priority substances in Member Sates.

A method called the EU Risk Ranking Method (EURAM) is used to handle the large amounts of information in IUCLID. The EURAM is a simple screening[7] tool for ranking and scoring chemicals based on risk assessment principles. Human health and environment scores are calculated, each based on an exposure and an effects score. Initially EURAM generates an automated ranking of substances based on IUCLID data.

[7] The EURAM Method is not a "mini" risk assessment but is intended to summarize the vast amounts of information in IUCLID.

The Regulation outlines factors that should be taken into account when drawing up the EU priority lists. These are:

- The effects of the substance on humans or the environment;
- The exposure of man or the environment to the substance;
- The lack of data on the effects of the substance on man and the environment;
- Work already carried out in other fora;
- Other Community legislation and/or programs relating to dangerous substances.

There is also an Expert Judgement where the EU Commission leads meetings of Member States, Industry and NGOs to discuss the ranking and any unexpected anomalous results.

In the third step, substances on the priority list undergo an in-depth risk assessment. The assessment covers:

- Risks posed by the priority chemical to humans (workers, consumers and human exposure via the environment)
- Risks posed by the priority chemical to the environment (the terrestrial, aquatic and atmospheric ecosystems and accumulation through the food chain).

The fourth step involves actions to reduce the risks posed by the priority substance, as determined by the risk assessment.

Data Requirements

The data that is required to be submitted to the Commission on HPVCs includes:

- Name of the substance;
- Produced and/or imported quantities;
- Classification and labelling information under Directive 67/548;
- Reasonably foreseeable uses;

Furthermore, the Regulation requires that available data in the following areas be submitted:

- Physico-chemical properties;
- Information related to chemical fate and pathways;
- Toxicological and ecotoxicological properties.

Sources of Input Data

Companies are obliged by Regulation 793/93 to make every reasonable effort to obtain information on HPVCs that they produce or import. All companies that submit data are required to update the information every three years at a minimum.

Outcomes

For each substance, a Member State is appointed to act as rapporteur for the risk assessment and write the first draft of the risk assessment reports. The Commission mediates meetings during the assessment and after publication of the draft, which attempt to reach consensus on the conclusions of the risk assessments. Steps to reduce risk are taken, if the risk assessment concludes that "further risk reduction measures, beyond those already in place, are required". If so, a risk reduction strategy is developed.

Resources Required

The overall process is resource intensive, although the use of EURAM reduces the amount of resources that would be necessary. Companies can combine their efforts for data submission and reduce the amount of resources they need to submit the required data.

Constraints

The ranking produced by EURAM is largely based on acute and chronic aquatic toxicity data. There is little data available on other types of toxicity. The ranking scores tend to form groups that are not very well differentiated – this is a result of using default "worst-case" input data when better data is not available.

Example of Use

Octa-bromo-diphenylether was listed on the first priority list based on the information that was available on this substance. The U.K. and France were the rapporteur countries for this chemical. The subsequent risk assessment resulted in the establishment of a strategy for limiting the risks associated with this substance.

Sources

European Chemicals Bureau. Existing Chemicals. http://ecb.jrc.it/existing-chemicals/

Hansen, Bjorn G. et al. *Priority Setting for Existing Chemicals: European Union Risk Ranking Method.* Environmental Toxicology and Chemistry. Vol. 18, No. 4, pp. 772-779. 1999. SETAC Press.

van Haeslt, Anniek G. and Bjorn G. Hansen. Priority Setting for Existing Chemicals: Automated Data Selection Routine. Environmental Toxicology and Chemistry. Vol. 19 No. 9, pp. 2372-2377. 2000. SETAC Press.

German Existing Chemicals Evaluation

Prioritization Function

Scan and Scope
Screen
Characterization
Score

Description

The Advisory Committee on Existing Chemicals (BUA) of the German Chemical Society uses a priority setting method in order to set priority lists of existing chemicals for evaluation. Initially, the list of approximately 100,000 existing chemicals was reduced to about 1100 chemicals that are produced in amounts greater than 1000 tonnes per year. Of these 1100 chemicals, examination of a number were postponed:

- Pesticides and pharmaceuticals, as they are covered under other regulations
- Inorganic substances, in particular heavy metal compounds, since comprehensive data already exists
- Substances of mainly natural origins, such as amino acids
- Chemicals that are not stable in the environment, such as acid chlorides

These exclusions brought the list down to 780 chemicals. For these chemicals, industry was required to provide toxicological and ecotoxicological information in the form of an abbreviated data set.

BUA used these data sets to categorize the substances based on their toxicity, ecotoxicity, biodegradability and exposure. The substances are divided into four categories:

- Group I: Substances having a risk potential for humans and the environment
- Group II: Substances with insufficient data
- Group III: Substances with low risk potential
- Group IV: Substances with a risk potential only at the workplace

Data Requirements

The initial data set submitted by industry must include toxicological and ecotoxicological data.

Sources of Input Data

Initially the chemicals industry provides all existing toxicological and ecotoxicological data and any internal company information in the form of an abbreviated chemical data set. The minimum required data set was established and agreed upon by the Chemical Industry Association and the Federal Ministry for the Environment, Nature Protection and Reactor Safety. After the prioritization takes place, further information is gathered depending on the group classification.

For Group I comprehensive reports, the largest manufacturer or importer of the chemical in question must conduct a literature search to compile all existing data on the chemical. In the case of Group II substances, BUA recommends further testing that must be carried out by industry.

Outcomes

The prioritization process results in the distribution of existing chemicals into the four categories mentioned above. Chemicals in Group I are the subject of a comprehensive report by BUA. These reports are used as a basis for government agencies to conduct risk evaluations, which may result in risk management and risk reduction measures. Substances in Group II must be further studied in order to designate them as being Group I, Group III or Group IV. Group III chemicals are the subject of a short report by BUA. Substances in Group IV are recommended for study by the BG Chemie (Employment Accident Insurance Fund of the Chemical Industry).

Resources Required

This process is fairly resource intensive for industry, in particular for Group II chemicals that require additional testing. The amount of time required is also dependent of the knowledge level of the participants.

Constraints

This methodology excludes a number of different types of chemicals as mentioned above. Also, certain physical parameters of the testing procedures, such as temperature, mean that the test results would not be universally applicable (e.g. the results wouldn't apply in an arctic environment). Finding exposure data and obtaining internal company studies also pose a challenge.

Sources

Advisory Committee on Existing Chemicals (BUA) (1999): *Assessment of Existing Chemicals*. Chapter V: National Assessment of Existing Chemicals with Production Volumes Exceeding 1000 t/a, p. 18-33.

Greim, Heidrun, German Advisory Committee on Existing Chemicals (BUA), Personal communication, February 2004

Health Effects Indicator Decision Index (HEIDI)

Prioritization Function

Screening
Characterization
Scoring and Ranking

Description

The Network for Environmental Risk Assessment and Management (NERAM) developed HEIDI as part of the National Framework for Petroleum Refinery Emission Reductions (NFPRER) initiative. The tool is a spreadsheet-based screening-level tool to assist policymakers in prioritizing reductions of air emissions from Canadian petroleum refineries on the basis of estimated risk to human health. The tool produces rankings of the potential health impacts associated with three classes of air emissions: (1) carcinogenic air toxics (2) non-carcinogenic air toxics, and (3) criteria air contaminants (CACs) using available data for each of the 20 refineries in Canada in a generic emission model. HEIDI provides relative rankings of the estimated health impacts associated with the three classes of substances based on predicted incidence of health effects, as well as a summary health measure that allows for a comparative ranking based on the combined incidence and severity of health effects.

Data Requirements

The user of the tool must select the refinery scenario (a refinery in a certain location or a "worst-case" refinery), enter the mixing height of pollutants, and the reduction targets for emissions. The user must also enter information about the refinery: the mass of refinery emissions, stack height and velocity, etc.

Sources of Input Data

The refinery scenario may be selected to approximate an existing refinery. Some inputs have a default value (e.g. the mixing height default is 1.5 km). Refinery emissions data would probably be the same data that is required for the National Pollutant Release Inventory (NPRI). Other data necessary for the models, such as characteristics of the pollutants, are embedded in the tool.

Outcomes

HEIDI provides the following three health impact ranking outputs:

1) Ranking of pollutants based on predicted number of annual cases of health effects.
2) Ranking of pollutants based on simplified Disability Adjusted Life Years (DALYs) that provide a common measure for comparing the severity of different health endpoints (e.g. cancer, non-cancer illnesses, and cardiorespiratory illness and death).
3) Ranking of pollutants based on more complex Disability Adjusted Life Years (DALYs) that consider the severity of illness, age of onset, and the reversibility of harm.

The number of cases health effects or DALYs is shown as a percentage of the total cases or DALYs within each category of chemicals.

Resources Required

This tool requires a relatively moderate amount of time and effort. Much of the emissions data required would probably be available from government-required reporting.

Constraints

As with any model, there is significant uncertainty associated with the outcomes. The outcomes are the result of rough statistical estimates of predicted incidence rates for a variety of health endpoints of widely differing severity. The results are thus useful for comparing the relative estimated health impacts, but do not represent absolute estimates of health risks.

Example of Use

This tool was developed specifically for the Canadian petroleum refinery industry, and has been assessed by the NFPRER Health Prioritization sub-group for inclusion in the National Framework for Petroleum Refinery Emission Reductions.

Sources

National Framework for Petroleum Refinery Emission Reductions Steering Committee and National Air Issues Coordinating Committee - Other Air Issues. *National Framework for Petroleum Refinery Emission Reductions: Discussion Document*. Feb. 3, 2004.

McColl, R.S., Hicks, J. Shortreed, J.S. and Craig, L. *Health Effects Indicator Decision Index (HEIDI): A risk-based tool for ranking abatement of air pollution release inventories by expected regional health effects* (poster).

CCME (2003): Steve McColl, John Hicks, Lorraine Craig, John Shortreed (NERAM): Assessment of Comparative Human Health Risk-based Prioritization Schemes for Petroleum Refinery Emission Reductions. Prepared for CCME National Framework for Petroleum Refinery Emissions (NFPRER) Health Prioritization Sub-Group, Final Report (May 26, 2003). Available at http://www.irr-neram.ca/pdf_files/CCME1.pdf

Intake Fraction for Multimedia Pollutants

Prioritization Function

Characterization

Description

The adverse affects of a chemical depend on the intake of all exposed individuals and the likelihood of adverse affects with increased intake. This methodology looks specifically at the intake, which depends on the transport and fate of the chemical and the human exposure.

Intake fraction is the fraction of a chemical mass emitted into the environment that eventually passes into a member of the population through inhalation, ingestion, or dermal exposure. To date, this concept has been primarily applied to pollutants whose primary route of exposure is inhalation. However, Bennett et al[8] have demonstrated its use for multiple exposure pathways. For their calculation of intake fractions, they employed the CalTOX multimedia fate and exposure model. This type of modeling is able to provide a fairly large amount of differentiation between chemicals.

Data Requirements

This type of modeling requires many properties of the chemical, including basic chemical properties (molecular weight, vapour pressure, melting point), partition co-efficients in various media, biotransfer factors and reaction half-lives.

Sources of Input Data

The necessary data was available in the CalTOX model. CalTOX contains the chemical properties needed for fate and exposure modeling for over 300 chemicals.

Outcomes

Intake fractions can classify chemicals by their dominant pathway i.e. inhalation dominant, ingestion dominant, dermal dominant or multipathway. Separate intake fractions can be calculated for releases to air and to water. Intake fractions can also be used with different transport and fate models to show the similarities and differences between the models.

Resources Required

The amount of resources needed to complete the modeling is not clear. Using available data, it would probably require a moderate amount of resources to determine intake fractions.

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[8] Bennett, Deborah H., Margni, Manuele D , McKone, Thomas E., and Jolliet, Olivier (2002). Intake Fraction for Multimedia Pollutants: A Tool for Life Cycle Analysis and Comparative Risk Assessment. Risk Analysis 22, no.5, 905-918

Constraints

An extensive amount of fate and exposure data is required for this type of modeling, which may not be available for all chemicals.

Example of Use

In Bennett et al, the authors calculated air and water intake fractions for 308 organic chemicals on the US EPA Toxic Release Inventory List.

Sources

Bennett, Deborah H., Margni, Manuele D., McKone, Thomas E., and Jolliet, Olivier (2002). Intake Fraction for Multimedia Pollutants: A Tool for Life Cycle Analysis and Comparative Risk Assessment. Risk Analysis 22, no.5, 905-918.

Multiple Issue Contribution

Prioritization Function

Score
Rank and Cluster

Description

Multiple Issue Contribution is a methodology for combining different quantitative indicators of environmental impact or performance. For example, a chemical may be assigned certain values for global warming potential and ozone depletion potential. The Multiple Issue Contribution method would allow these measures to be combined into a single score.

Initially, the environmental impacts must be normalized. This is accomplished by dividing the impact under consideration by a reference amount, which, for example, may be the total impact in the province, country or world. The normalization results in a unitless number (e.g. % contribution to total impact in region, country or world).

The weighting factors that are used in the method are explicitly based on value-choices, and are therefore intentionally subjective and value-laden. This process can include the additional step of aggregating the weighted indicator results into a single score.

The basis for the weighting step can be different value systems from different origins. Weighting can be based on national policy, social and societal preferences, a company's policy, political, or individual preferences. Possible sources include:

- Sustainable development guidelines;
- Environmental policy targets (short or long term targets);
- Public opinion polls;
- Expert polls or
- Company targets.

The relevance of the individual environmental issues, in this method, is expressed by weighting the related impact categories using scores. Commonly a weighting between 1 and 10, where 10 represents an impact felt to be very important and 1 an impact considered not important is used.

Data Requirements

This method requires characterization factors for all the impacts that are deemed to be important according to the subjective weighting scheme. It also requires normalization factors for each of these impacts.

Sources of Input Data

Impact category factors for individual materials and chemicals can be obtained from databases such as CML (the Leiden University's Institute of Environmental Sciences) or the US EPA's TRACI (Tool for the Reduction and Assessment of Chemicals and other environmental Impacts). Normalization factors are also available from CML.

Outcomes

This method is generally used to compare different product designs, but might be used for individual chemicals. The outcome is a list of weighted impacts, which may be combined into a single score. The single score allows the items (e.g. chemicals, product designs) to be compared on the basis of all of the impacts simultaneously.

Resources Required

The establishment of a weighting scheme to reflect values may be a major undertaking, such as a meeting of experts or a public poll, or may use a simpler approach such as a scheme based on government policy. The weighting of impacts and ranking of alternatives does not require a great deal of resources.

Constraints

This process is inherently subjective in nature, and as such it must be done carefully so that it is fully transparent. A clear explanation must be given of how the weighting scheme was developed and who developed it.

Example of Use

The Multiple Issue Contribution process was employed in a Design for Environment case study that was led by Five Winds International, Magna International Inc, and Intier Automotive Inc., in partnership with the Automotive Parts Manufacturers Association, 3M Canada, the University of Waterloo, Natural Resources Canada and Industry Canada. The case study involved a Life Cycle Assessment conducted on an automotive door panel. The possible designs were analyzed using LCA software and the results were ranked using a weighting scheme developed by an expert panel. The panel consisted of a group of experts from industry and public policy who were assembled and asked to consider and weight a list of impact categories based on their propensity to contribute to environmental sustainability as defined by the Brundtland Commission. As a sensitivity analysis, the ranking process was also carried out utilizing a different weighting scheme. This scheme is based on surveyed opinions of the general population of individuals in Europe, carried out by the European Statistics Bureau, on which issues contribute most to environmental sustainability in Europe. This additional analysis was carried out to compare the final results of both weighted evaluations.

Sources

Five Winds International et. al. DfE Case Study: Applying design-for-environment & eco-efficiency in auto parts manufacturing. 2001. Available from Five Winds International.

Persistence, Bioaccumulative and Toxic (PBT) Profiler

Prioritization Function

Screen
Characterization

Description

The PBT Profiler is a methodology for screening chemicals and materials for persistence, bioaccumulation and toxicity. The approach is implemented by means of a subset of estimation methods included in the U.S. EPA's Office of Pollution Prevention and Toxic's P2 Framework. The PBT Profiler was developed jointly by EPA, The American Chemistry Council, The Chlorine Chemistry Council, the Synthetic Organic Chemical Manufacturers Association and with the support and contributions of Environmental Defense. It is publicly available online, for no cost. The PBT Profiler is a component of the EPA's PBT Chemical Program, which is intended to provide a new approach to reducing risks from and exposures to priority PBT chemicals through increased coordination among EPA national and regional programs.

Data Requirements

For this preliminary screening tool a low level of data is required. A user enters a chemical name, CAS (Chemical Abstract Service) registry number (if available), and the chemical structure. The user may use a drawing program to draw and enter the structure, or the structure can be entered as a SMILES Notation. SMILES is the Simplified Molecular Input Line Entry System. It is a chemical notation system used to represent a molecular structure by a linear string of symbols.

Sources of Data

Chemicals are assessed in the PBT Profiler using structure-based estimation methods. Several different models are applied to the chemical structure to produce estimates of persistence, bioaccumulation and toxicity.

Outcomes

The profiler gives approximate measures of persistence in water, sediment, soil and air in days. Bioaccumulation is represented by an estimated bioconcentration factor, and toxicity is represented by an estimation of chronic toxicity to fish in mg/l. The profiler also indicates whether the results exceed EPA criteria for persistence, bioaccumulation and toxicity.

Resources Required

The use of the PBT Profiler requires very few resources. It provides an easy method of early level chemical screening.

Constraints

The EPA stresses the use of this tool as a screening method only, to be used for identifying areas of potential concern. There are many chemicals that cannot be assessed using the PBT Profiler: chemicals with experimental data, inorganic chemicals, reactive chemicals, most organic salts, high molecular weight compounds, chemicals with unknown or variable composition, mixtures, surfactants and highly fluorinated compounds.

Example of Use

SC Johnson has worked extensively with the EPA and entered information on its raw materials into the PBT Profiler. The Profiler has been explicitly designed so that it can be used anonymously, and as such data on other users could not be obtained.

Sources

US EPA. Persistence, Bioaccumulative and Toxic (PBT) Profiler.
http://www.epa.gov/oppt/pbtprofiler/

US EPA. Persistent Bioaccumulative and Toxic (PBT) Chemical Program. 2003.
http://www.epa.gov/opptintr/pbt/index.htm

RSEI: Risk Screening Environmental Indicators

Prioritization Function

Screening
Characterization

Description

In response to the need for environmental indicators, and to take advantage of the rich data source offered by the Toxics Release Inventory (TRI), the Office of Pollution Prevention and Toxics (OPPT) convened a workgroup to explore the development of an indicator or indicators based on the TRI that could track changes in human health and environmental impacts better than reports of pounds of releases alone. Specifically, the approach would integrate toxicity, exposure and population considerations into the evaluation of releases. The Risk-Screening Environmental Indicators method was developed in response to this initiative.

The RSEI approach is very flexible and can be implemented in various ways. Modeled exposures and effects can either be acute or chronic, and the potential impacts estimated can be on human health or on ecosystems. National, regional or local emissions databases can be used. The use of the model is not limited to TRI chemicals; in principle, the adaptable method can model any chemical if toxicity characteristics, physicochemical properties, release levels, and release location are known or can be estimated.
The RSEI is a Windows based computer program that is available at no charge from the U.S. EPA.

RSEI considers the following information: the amount of chemical released, the location of that release, the toxicity of the chemical, its fate and transport through the environment, the route and extent of human exposure, and the number of people affected. This information is used to create numerical values that can be added and compared in limitless ways to assess the relative hazard and risk of chemicals, facilities, regions, industries, or many other factors. The numerical values are calculated as follow:

Risk-related results: Surrogate Dose x Toxicity Weight x Population
Hazard-based results: Pounds x Toxicity Weight
Pounds-based results: TRI Pounds released

Data Requirements

The user of the RSEI selects the chemicals of interest and the geographic region under study. The program then calculates the results using the appropriate data.

Sources of Input Data

Data on chemical toxicity, fate and transport, as well as exposure and the number of people affected are contained in the tool.

Outcomes

The RSEI provides three different types of results. The Risk-related result combines estimates of toxicity, exposure level, and the exposed population to provide risk-related comparisons for air and water releases. The Hazard-based result applies toxicity information to the number of pounds released and examines the results for all release pathways from a hazard-based perspective. In the Pounds-based result one can view the number of pounds released or transferred by a facility, as reported to the Toxics Release Inventory, for the release pathway being considered. The software also allows the user to display the results using tables, graphs, maps and air concentration plumes.

Resources Required

Since most of the data is contained in the RSEI database, and it performs all of the calculations, the RSEI can be used very quickly, in minutes or hours, to perform screening level analyses.

Constraints

RSEI does not provide users with a quantitative risk estimate (e.g., excess cases of cancer). In the current version of the model, only air and surface water exposures are fully modeled. RSEI does not evaluate individual risk. Full-risk related modeling is provided for the majority of TRI chemicals but excludes non-TRI chemicals. RSEI results have greater uncertainty when examining disaggregated results at the local or facility level. The model assumes that air concentrations of TRI chemicals are the same for indoor and outdoor exposures, and that populations are continuously exposed. Dermal and food ingestion pathways (other than fish consumption), and some other indirect exposure pathways are not evaluated. Ecological effects and acute health effects associated with short-term, periodic exposures to higher levels of these same chemicals are not addressed.

Additionally, RSEI contains only U.S. geographic and population data.

Example of Use

RSEI has been used for risk, compliance, and environmental justice analysis of Federal facilities reporting to TRI. It has also been used for industry sector- and facility-based targeting and strategic planning by several EPA offices. Outside analysts have investigated:

- impact of regulations on cross-media risk transfers;
- national environmental justice issues;
- community-based environmental protection;
- toxicity weights used for priority ranking at local level;
- assess disproportionate impacts on local population.

Sources

US EPA. Risk Screening Environmental Indicators. 2003.
http://www.epa.gov/opptintr/rsei/index.html

TRACI: Tool for the Reduction and Assessment of Chemical and other environmental Impacts

Prioritization Function

Characterization

Description

TRACI is an impact assessment tool that can be used with life cycle data. Life cycle data refers to information on all the inputs (energy, raw materials) and outputs (air emissions, solid waste) that occur in order to produce, transport, use and dispose of a product. The main purpose of TRACI is to help determine priorities or to make a preliminary comparison of two or more materials or product design options. However, the embedded database of characterization factors can be used to look at individual chemicals. The TRACI software is available for downloading from the EPA website. TRACI contains the following environmental impact categories:

- Ozone Depletion
- Global Warming
- Acidification
- Cancer
- Non-cancer
- Criteria Pollutants
- Eutrophication
- Smog Formation
- Ecotoxicity
- Fossil Fuel Use
- Land Use
- Water Use

Data Requirements

To look at individual chemicals, only the chemical name would be needed in order to look up specific impacts.

Source of Data

TRACI contains an embedded database of characterization factors for all the impacts mentioned above. The characterization factors can be exported from the TRACI software into Excel. It is then possible to look up the characterization factors for specific chemicals.

Outcomes

It is possible to determine impact characterization factors for a number of different impact categories for a given chemical, using the TRACI database.

Resources Required

In order to use TRACI it is necessary to download the program from the EPA website. The user would need to spend a couple of hours to become familiar with the program. To evaluate individual chemicals they would have to be entered into the program, or alternatively the list of characterization factors could be downloaded and the factors for the chemicals could be looked up manually.

Constraints

The use of TRACI to quantify impacts is limited to the inventory of chemicals that are included in the database. This varies widely in the different impact categories, from just a few to several hundred.

Example of Use

TRACI is intended for use by companies, federal facilities, industrial organizations and public interest groups. The National Institute of Standards and Technology has made use of the TRACI characterizations factors in their Building for Environmental and Economic Sustainability (BEES) software. TRACI is being utilized in two EPA Office of Pollution and Prevention and Toxic programs: Design for Environment and Environmentally Preferable Products. It is also being incorporated into the SimaPro life cycle software, and being used in academic curricula and used in industry work, such as Nexant's case study on ultra-clean fuel types.

Sources

US EPA. National Risk Management Research. TRACI - Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts. 2002.
http://www.epa.gov/ORD/NRMRL/std/sab/iam_traci.htm

Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI): User's Guide and System Documentation. US EPA. 2002.

Lippiatt, B.C., NIST. BEES Technical Manual and User Guide. 2002.

Bare, J. Personal communication. May 28, 2003.

APPENDIX 3: OECD DATABASE OF CHEMICAL RISK ASSESSMENT MODELS

In 2001/2002 the OECD (Organization for Economic Cooperation and Development) surveyed OECD Member countries about what chemical risk screening models they use and in what context they use these models. The information collected was published in a searchable database available on the Internet.[9] Although the database does not contain all models being used and is not updated regularly, it provides an interesting "snap shot" of the range of chemical risk screening models being used in OECD countries. Box 1 shows the OECD's own description of and disclaimer about this database. The following table shows the range of properties and effects covered by the various models in the database.

Box 1: OECD database of Chemical Risk Screening Models

This searchable database includes information on models (computerised or capable of being computerised) that are used by OECD Member governments and industry to predict health or environmental effects (e.g., QSARs), exposure potential and possible risks. The methods described here have not been evaluated or validated by OECD, and no endorsement of the methods by OECD should be inferred by the inclusion of certain methods in this database.

This database is intended as an information resource only, and is not intended to present a comprehensive evaluation of these methods. OECD is not recommending these methods as being the best or only methods available. The users should conduct their own investigation of the methods to determine if the methods are appropriate for the user's chemicals and/or situation.

The methods described here are screening level methods that should be used only in the absence of data. Any screening level method should be used with caution because screening level methods have inherent limitations and uncertainties. The user should be familiar with the specific limitations and uncertainties of the method of interest. Measured data are always preferred over data predicted or estimated by screening level methods. Screening level methods are useful, when chemical-specific data are lacking, for establishing priorities for chemical evaluation and for identifying issues of potential concern.

Methods described here have not been evaluated or validated by OECD. No endorsement by OECD should be inferred by the inclusion of certain methods in this database.

Source: OECD, http://webdomino1.oecd.org/comnet/env/models.nsf

[9] Available at http://webdomino1.oecd.org/comnet/env/models.nsf

Properties and Effects Covered in OECD Model Database

Model Property	Property/Effects Modelled	Number of Models
Physical-Chemical Properties	Flash point, Heat of Vaporization, K_{oc}, K_{ow}, LogD, MP BP VP, pKa, WS	19
Human Health Hazard	Ames Mutagenicity, Developmental Toxicity, Mutagenicity, Neurotoxicity, Noncarcinogenic Chronic Hazard Index, Oncogenicity, Reproductive Toxicity, Sensitisation, Skin / Eye Irritation, Systemic Toxicity	7
Human Health Exposure / Risk: Routes of Exposure	Dermal, Ingestion, Ingestion of beef and dairy products, Inhalation, Multi-media	41
Human Health Exposure / Risk: Types of Exposure	Consumer product exposure, Direct exposure to contaminated environmental media, Exposure to soil contamination, Indirect human exposure via the environment, Intake of chemicals in food, Worker exposure	40
Environmental Hazard	Aquatic Biota, Terrestrial Biota	8
Environmental Fate Properties	Air soil water sediment concentrations, Air water concentrations, Air water sediment concentrations, AOP, BCF, Biodegradation, Concentrations in aquatic biota, Groundwater concentrations, Half-life in air, Henry's law constant (HLC), Hydrolysis, Metabolic pathways, Persistence, Persistence (regional), Photodegradation, Removal % in Wastewater Treatment, Stable biodegradation products, Toxic endpoints of biodegradation products, Volatilization from water	42
Environmental Exposure / Risk: Exposure Pathways	Air, Biota, Groundwater, Multi-media, Sediment, Sewage treatment plant, Sludge compartment, Soil, Water	35
Environmental Exposure / Risk: Biota Exposed	Fish- and worm-eating predators, Freshwater, Marine, Microorganisms in sewage treatment plant, Sediment, Terrestrial, Wetlands organisms	22
Total *Note column does not add due to overlap between properties*		104

The following simple screening criteria were used to identify models most likely to be relevant for setting priorities for ambient air quality objectives:

- Eliminate models that deal only with Physical-Chemical Properties or Environmental Fate Properties;

- Eliminate models clearly not relevant to ambient air quality objectives (e.g. soil contamination, drinking water, site-specific decision making, indoor air quality); and
- Eliminate models without documentation in English.

These screening criteria eliminated all but 13 of the models in the database. Detailed profiles of these 13 models were downloaded from the OECD database and are included in Appendix 4. Two of these models (ChemSTEER and PBT Profiler) are only profiled in Appendix 2. The scope of this project did not allow for further review of additional models.

APPENDIX 4: OECD CHEMICAL RISK ASSESSMENT MODELS

ChemCAN 4.0 Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		ChemCAN 4.0
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box.* Regulatory ( ) Research (X) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	(100 words Maximum) Health Canada – for estimation of human exposure concentrations in environmental media
3. Areas of assessment		*Please check the appropriate box.* Human health ( ) Environment (X)
4 Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment ( ) Consumer product exposure ( ) Worker exposure ( ) Not Applicable (X) Others. ( ) Comments.
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation ( ) Ingestion ( ) Dermal ( ) Multi-media ( ) Not Applicable (X) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (X) Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( )

		Fish-and-worm eating predators	( )
		Not Applicable	( )
		Others:	( )
		Comments: Bioconcentration factor is calculated	
	(b) Pathways of exposure covered	*Please check the appropriate box*	
		Air	(X)
		Water	(X)
		Sediment	(X)
		Soil	(X)
		Biota	(X)
		Sewage treatment plant	( )
		Multi-media	(X)
		Not Applicable	( )
		Others	( )
		Comments: Multi-media (air, water, soil and sediment) concentrations, regional environmental persistence of contaminant.	
6 Type of Information Provided		*Please check the appropriate box*	
		Daily intake	( )
		Potential dose	( )
		Margin of safety	( )
		Predicted environmental concentration	(X)
		Risk quotient (predicted environmental concentration / predicted no-effect concentration)	( )
		Others	(X)
		Comments: Bioconcentration factor is calculated	
7. Model Approach		Comments (100 words Maximum) Deterministic or Probabilistic	
1. Limitations of Model		(Max. 100 words) Not designed for site-specific assessments Applicable only to organics and non-speciating metals Evaluation exercises have focused on non-ionising organic chemicals	
2. Are limitations clearly described for user of Model?		(Max. 100 words) Appropriate use and limitations are discussed in the series of papers by Mackay et al. (1996 a,b,c).	
3. Which types of chemicals can appropriately be evaluated by the Model?		(Max. 100 words) non ionisable organics and non-speciating metals	
4. Which types of chemicals can NOT be evaluated by the Model?		(Max. 100 words) speciating metals (eg. mercury)	
1. In what written language is Model available?		(Max. 100 words) English	

2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		(Max 100 words) No (N/A)
3 Does the Model contain a searchable Database?		(Max. 100 words) Yes, of chemicals with physico-chemical properties, and of regional environmental parameters.
4. Is the Model Computerized?		(Max. 100 words) Yes – Windows Application.
1. Output / Information provided by the Model		(Max. 100 words) Outputs - media-specific concentrations - regional persistence - advective vs reactive removal of chemical
2. Input data needed to use the Model		(Max. 100 words) Inputs – physico-chemical properties of the chemical - environment characteristics estimated emissions
3. (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s)	(Max. 100 words) Shown at time of download http://www.trentu ca/envmodel/
	Is the User's Manual incorporated into help screens within the computer model?	(Max. 100 words) No
4. Computer hardware requirements		(Max. 100 words) Any Windows PC or Power Mac
5. Computer software requirements		(Max. 100 words) Microsoft Windows 3.1 or 95-98
6. Skill / Expertise / Training required to use the Model		(Max. 100 words) None
1. Has the Model been evaluated with data?		(Max. 100 words) Yes… MacLeod and Mackay (1999) Kawamoto, MacLeod and Mackay (2000)
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		(Max 100 words) Partially validated… Model has been shown to be a useful descriptor of chemical fate over a limited range of its possible applications.
3. Has the Model been published or peer reviewed? If so, provide citation(s)		(Max 100 words) Yes Mackay (1996 a,b,c)

4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).	(Max. 100 words) Application to the chlorobenzenes in southern Ontario - MacLeod and Mackay (1999) Application to 68 chemicals in Japan - Kawamoto, MacLeod and Mackay (2000)
1. Is the Model publicly available, or is it proprietary?	(Max. 100 words) Publicly available
If it can be downloaded from the Internet, what is the web address (URL)?	Yes… http://www.trentu ca/envmodel
2 How frequently is it updated?	(Max. 100 words) Model revisions every 2-3 years
3. How much does it cost to obtain the Model (if any)?	(Max. 100 words) Free.
1. Creator, Author or Sponsoring Organization	D. Mackay, A. Di Guardo, S. Paterson, D Tam
2. Country of Origin	Canada
3. Latest Version number and date of latest update / revision	4.0, May 1996 Database updated November 1997. Version 6.0 expected in July, 2000.
4. Identify previous versions or contributing elements (names and dates) of the Model	ChemCAN 1.0 ChemCAN 2.0
1. Name	Matthew MacLeod
2. Affiliation	Trent University
3. Department	Canadian Environmental Modelling Centre
4. Address	1600 Westbank Drive
5. Postal / Zip code	K9L 1Y7
6. City and Country	Peterborough, Ontario, Canada
7. Tel / Fax / Email	(705) 748-1011 X 5341 mmacleod@trentu.ca

Full Citations

Mackay D, Paterson, S., Kicsi, G., Di Guardo, A., Cowan, C.E. 1996a. Assessing the Fate of New and Existing Chemicals: A Five Stage Process. Environ. Toxicol. Chem. 15: 1618-1626.

Mackay D, Paterson, S., Di Guardo, A., Cowan, C.E. 1996b. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15: 1627-1637.

Mackay D, Paterson, S., Kicsi, G., Cowan, C.E., Di Guardo, A., Kane, D.M. 1996c. Assessment of Chemical Fate in the Environment Using Evaluative, Regional and Local-Scale Models:

Illustrative Application to Chlorobenzene and Linear Alkylbenzene Sulfonates. Environ. Toxicol. Chem. 15: 1638-1648.

MacLeod, M., Mackay, D. 1999. An assessment of the environmental fate and exposure of benzene and the chlorobenzenes in Canada. Chemosphere 38: 1777-1796.

Kawamoto, K., MacLeod, M., Mackay, D. Evaluation and Comparison of Mass Balance Models of Chemical Fate: Application of EUSES and ChemCAN to 68 Chemicals in Japan. Chemosphere. (In Press, 2000)

CHEMFRANCE Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		CHEMFRANCE
2 Purpose / Use of Model	(a) Purpose	*Please check the appropriate box:* Regulatory (X) Research ( ) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	Chemfrance is designed to support decision-making by risk managers in the government, scientific institutes and industry in the evaluation of chemical substances in France.
3. Areas of assessment		*Please check the appropriate box:* Human health ( ) Environment (X)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment ( ) Consumer product exposure ( ) Worker exposure ( ) Not Applicable ( ) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation ( ) Ingestion ( ) Dermal ( ) Multi-media ( ) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (X) Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others ( )

		Comments:
	(b) Pathways of exposure covered	*Please check the appropriate box* Air (X) Water (X) Sediment (X) Soil (X) Biota (X) Sewage treatment plant ( ) Multi-media (X) Not Applicable ( ) Others: ( ) Comments:
6. Type of Information Provided		*Please check the appropriate box* Daily intake ( ) Potential dose ( ) Margin of safety ( ) Predicted environmental concentration (X) Risk quotient (predicted environmental concentration / predicted no-effect concentration) ( ) Others: ( ) Comments:
7. Model Approach		Comments Computer model allowing to estimate the environmental fate of chemicals in France. The outputs of the model consist of estimated chemicals distribution between environmental media, transport and transformation process rates, and steady state concentration in one of the twelve defined region in France, or France as a whole, at a chosen season
1. Limitations of Model		☐ A model is always a «cartoon of reality» ☐ Expertise of user is important: data evaluation (garbage in, garbage out), interpretation of results ☐ Model analyses (incl. Validation) has been performed to a limited extent ☐ The model results can be unreliable when expertise is lacking
2 Are limitations clearly described for user of Model?		NO
3. Which types of chemicals can appropriately be evaluated by the Model?		Organic chemicals
4. Which types of chemicals can NOT be evaluated by the Model?		Inorganic chemicals, Metals, dissociating chemicals
1. In what written language is Model available?		French
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		No

3 Does the Model contain a searchable Database?		No
4. Is the Model Computerized?		Yes
1. Output / Information provided by the Model		Print-out
2. Input data needed to use the Model		Physico-chemicals properties of the substance (same as level III fugacity model)
3. (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s).	- Devillers, J., Bintein, S. and Karcher, W (1995). CHEMFRANCE: A regional level III fugacity model applied to France. Chemosphere 30, 457-476. - Bintein, S. and Devillers, J. (1996) Evaluating the environmental fate of atrazine in France. Chemosphere 32, 2441-2456 - Bintein, S and Devillers, J (1996). Evaluating the environmental fate of lindane in France. Chemosphere 32, 2427-2440. - Devillers, J., Bintein, S. and Domine, D (1997). Modeling the environmental fate of atrazine. SAR QSAR Environ. Res 6, 63-79.
	Is the User's Manual incorporated into help screens within the computer model?	No
4 Computer hardware requirements		80386 DX processor (25 MHz), 4 Mb RAM, VGA display,
5. Computer software requirements		DOS
6. Skill / Expertise / Training required to use the Model		Expertise is required CHEMFRANCE is designed for skilled risk managers in government agencies, scientific institutes and industry.
1. Has the Model been evaluated with data?		Only to a limited extent
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		Algorithm validation and software evaluation have been performed. Numerical validation activities for parts of EUSES (modules or submodels) have been performed by comparison with measured data for several chemicals from different chemical classes.
3. Has the Model been published or peer reviewed? If so, provide citation(s).		- Devillers, J., Bintein, S. and Karcher, W (1995). CHEMFRANCE: A regional level III fugacity model applied to France. Chemosphere 30, 457-476.

4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s)	- Bintein, S. and Devillers J. (1996). Evaluating the environmental fate of atrazine in France. Chemosphere 32, 2441-2456 - Bintein, S. and Devillers, J. (1996). Evaluating the environmental fate of lindane in France Chemosphere 32, 2427-2440. - Devillers, J., Bintein, S and Domine, D. (1997) Modeling the environmental fate of atrazine. SAR QSAR Environ. Res 6, 63-79.
1 Is the Model publicly available, or is it proprietary?	Yes, publicly available
If it can be downloaded from the Internet, what is the web address (URL)?	
2. How frequently is it updated?	Every 5 years
3. How much does it cost to obtain the Model (if any)?	FREE
1. Creator, Author or Sponsoring Organization	CTIS, 3 Chemin de la Graviere,69140 Rillieux La Pape, France Authors : A. Chancrogne, S Bintein, D. Domine, J. Devillers Granted by the French Ministry of the Environment.
2 Country of Origin	FRANCE
3. Latest Version number and date of latest update / revision	CHEMFRANCE Version 2.0 (Octobre 1996)
4 Identify previous versions or contributing elements (names and dates) of the Model	CHEMFRANCE Version 1.0 (Octobre 1991)
1. Name	James Devillers, Ph.D
2. Affiliation	CTIS
3. Department	
4. Address	3 Chemin de la Graviere
5. Postal / Zip code	69140
6. City and Country	Rillieux La Pape, FRANCE
7. Tel / Fax / Email	Phone : +33 (0)4 7808 49 84 Fax : +33 (0)4 78 08 56 37 E-mail : jde-ctis@imaginet fr

CSOIL Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		CSOIL
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box* Regulatory (x) Research (x) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	CSOIL is used by the National Institute of Pubic Health and the Environment by order of the Ministry of Housing, Physical planning and the Environment. It is an Excel-spreadsheet program.
3. Areas of assessment		*Please check the appropriate box* Human health (x) Environment ( )
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (x) Consumer product exposure (x) Worker exposure ( ) Not Applicable ( ) Others: ( ) Comments: exposure due to soil contamination
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (x) Ingestion (x) Dermal (x) Multi-media (x) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms ( ) Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others: ( ) Comments.
	(b) Pathways of exposure covered	*Please check the appropriate box* Air (x) Water (x) Sediment ( )

		Soil	(x)
		Biota	(x)
		Sewage treatment plant	( )
		Multi-media	( )
		Not Applicable	( )
		Others:	( )
		Comments:	
6. Type of Information Provided		*Please check the appropriate box*	
		Daily intake	(x)
		Potential dose	(x)
		Margin of safety	( )
		Predicted environmental concentration	( )
		Risk quotient (predicted environmental concentration / predicted no-effect concentration)	( )
		Others:	( )
		Comments:	
7. Model Approach		Comments Based on the Maximum permissable Risk (TDI and 10-4 lifelong cancer risk) and exposure relations between soil and humans a (potential) risk limit for soil is derived by back calculation. Based on the soil concentration also the potential exposure can be calculated.	
1. Limitations of Model		Potential exposure is calculated, for site specific risk assessment adjustments are necessary It is not designed for site-specific risk assessment Expertise of user is important: data evaluation (garbage in, garbage out), interpretation of results Uncertainty analyses has been performed Validation is Certain process formulations are based on limited research and need to be improved The risk resulting from use of pesticides and biocides are not considered	
2. Are limitations clearly described for user of Model?		To a certain extent in 2 reports: Van den Berg, 1995; Visen berg en Swartjes, 1996) A manual is not yet available.	
3. Which types of chemicals can appropriately be evaluated by the Model?		metals and organic compounds (when toxicological and compound specific data are available)	
4 Which types of chemicals can NOT be evaluated by the Model?		other anorganic compounds then metals	
1. In what written language is Model available?		english	
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		No	
3. Does the Model contain a searchable Database?		Yes excel spreadsheet	
4. Is the Model Computerized?		Yes	

1. Output / Information provided by the Model		Yes
2. Input data needed to use the Model		compound specific data (i e. solubility, logKow, logKoc, Vapour pressure, Kp, BCF-plants) and toxicological risk limit For about 100 compounds available in data file
3. (a) Are References or User's Manual provided for User?		Yes (x) No ()
(b) If YES	Provide citation(s).	Reference: Van den Berg, R. (1995). Exposure of man to soil contamination A qualitative and quantitative analysis, resulting in proposals for human-toxicological C-Values (revision of the 1991 and 1994 reports). RIVM report 725201011. RIVM, Bilthoven, The Netherlands.
	Is the User's Manual incorporated into help screens within the computer model?	No
4. Computer hardware requirements		Minimal. 80486 DX processor (75 MHz), 4 Mb RAM, VGA display, Fixed drive with 10 Mb available, mouse. Recommended: 80486 DX or Pentium processor (>50MHz) and >8 Mb RAM
5. Computer software requirements		Windows 95 or windowsNT with Excel97
6. Skill / Expertise / Training required to use the Model		experience with excel 97
1. Has the Model been evaluated with data?		Only in uncertainty and sensitivity analysis Vissenberg, H.A. and F.A. Swartjes (1996) Evaluation of the exposure calculated with CSOIL by the performance on a Monte Carlo based sensitivity and uncertainty analysis. RIVM report 715810018 (in Dutch). RIVM, Bilthoven, The Netherlands
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		No
3. Has the Model been published or peer reviewed? If so, provide citation(s).		Model application is published in: Swartjes, F.A. (1999). Risk-based Assessment of Soil and Groundwater Quality in the Netherlands: Standards and Remediation Urgency. Risk Analysis 19, No 6: 1235-1249.
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		No
1. Is the Model publicly available, or is it proprietary?		No, currently only for research purposes and deriving guideline values
	If it can be downloaded from the Internet, what is the web address (URL)?	

2. How frequently is it updated?	when new data available, last update in 2000
3. How much does it cost to obtain the Model (if any)?	n.a.
1. Creator, Author or Sponsoring Organization	National Institute of Pubic Health and the Environment (RIVM)
2. Country of Origin	The Netherlands
3. Latest Version number and date of latest update / revision	june 2000
4. Identify previous versions or contributing elements (names and dates) of the Model	
1. Name	P.F. Otte
2. Affiliation	National Institute of Pubic Health and the Environment
3. Department	Laboratory of Soil an Groundwater research
4 Address	P.O. Box 1
5 Postal / Zip code	3720 BA
6. City and Country	BILTHOVEN, The Netherlands
7 Tel / Fax / Email	++31-30 2743965 ++31-302744419 PF.otte@rivm.nl

DRAFT Endocrine Disruptor Priority Setting Database, version 2 (EDPSDv.2)

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		DRAFT Endocrine Disruptor Priority Setting Database, version 2 (EDPSDv.2)
2 Purpose / Use of Model	(a) Purpose	*Please check the appropriate box:* Regulatory ( ) Research ( ) Others: Priority Setting (X)
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	Under development by USEPA to set priorities for testing of existing chemicals for endocrine-disruption potential, as required by the US Food Quality Protection Act of 1996. Use not anticipated until 2001
3. Areas of assessment		*Please check the appropriate box:* Human health (X) Environment (x)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (x) Consumer product exposure (x) Worker exposure (x) Not Applicable ( ) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (x) Ingestion (x) Dermal (x) Multi-media (x) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (x) Marine organisms (x) Sediment organisms ( ) Terrestrial organisms (x) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others: ( )

		Comments:
	(b) Pathways of exposure covered	*Please check the appropriate box*
		Air (x)
		Water (x)
		Sediment (x)
		Soil (x)
		Biota ( )
		Sewage treatment plant ( )
		Multi-media (x)
		Not Applicable ( )
		Others: ( )
		Comments:
6. Type of Information Provided		*Please check the appropriate box*
		Daily intake ( )
		Potential dose ( )
		Margin of safety ( )
		Predicted environmental concentration ( )
		Risk quotient (predicted environmental concentration / predicted no-effect concentration) ( )
		Others. Biological monitoring data, Measured environmental concentrations, Frequency of chemical detection, Chemical amounts (X)
		Comments:
7 Model Approach		Comments This priority setting strategy uses a database of compartmentalized exposure and effects-related information, as well as a category of specially targeted priorities. In this compartment-based approach, chemicals with similar data are compared to each other.
1. Limitations of Model		At present, only chemicals that are both High Production Volume and pesticide inerts are ranked; no assessment of risk; contains primarily secondary information sources of diverse quality
2. Are limitations clearly described for user of Model?		Limitations are described in Welcome New User section and in data source summaries
3. Which types of chemicals can appropriately be evaluated by the Model?		Currently, only chemicals that are both High Production Volume and pesticide inerts in the US can be ranked.
4. Which types of chemicals can NOT be evaluated by the Model?		Non-HPV/Inerts
1. In what written language is Model available?		English
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		No
3. Does the Model contain a searchable Database?		Yes
4. Is the Model Computerized?		Yes

1 Output / Information provided by the Model		Comma-separated values (CSV) export file or print-outs
2. Input data needed to use the Model		Default data scenarios; or Preloaded data customized by user via What-if capabilities; or Imported pre-ranked data containing only a (non-dashed) CAS number column and a numeric rank column, all as CSV data.
3. (a) Are References or User's Manual provided for User?		Yes (x) No ( )
(b) If YES	Provide citation(s).	See section F.1
	Is the User's Manual incorporated into help screens within the computer model?	Yes
4. Computer hardware requirements		Minimal requirements: Pentium II or better CPU, 32MB RAM, 75MB free disk space, monitor resolution at least 800 x 600 pixels
5. Computer software requirements		Windows 95 or newer
6. Skill / Expertise / Training required to use the Model		Some training or practice required to use EDPSDv.2, expertise required to interpret results (some sorting of chemicals for more advanced testing or exemption will be done after ranking)
1. Has the Model been evaluated with data?		NA
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		NA
3. Has the Model been published or peer reviewed? If so, provide citation(s).		No
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s)		
1. Is the Model publicly available, or is it proprietary?		A draft version of EDPSDv.2 was made publicly available in a June 2000 workshop for purposes of receiving comments.
	If it can be downloaded from the Internet, what is the web address (URL)?	www.ergweb.com/endocrine
2. How frequently is it updated?		
3. How much does it cost to obtain the Model (if any)?		NA
1. Creator, Author or Sponsoring Organization		USEPA
2. Country of Origin		USA
3 Latest Version number and date of latest		Version 2 Beta, May 22, 2000

update / revision	
4. Identify previous versions or contributing elements (names and dates) of the Model	See section F.1
1. Name	Conrad Flessner Jr.
2. Affiliation	USEPA
3. Department	Office of Pollution Prevention and Toxics
4. Address	1200 Pennsylvania Avenue, (7406)
5. Postal / Zip code	20460
6. City and Country	Washington, DC; USA
7. Tel / Fax / Email	Fax. 1 202 260 0981; e-mail: flessner.conrad@epa.gov

E-FAST Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		E-FAST
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box* Regulatory (X) Research ( ) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	Used by the U.S Environmental Protection Agency/Office of Pollution Prevention and Toxics. For assessment of New and Existing chemicals. Computerized model which provides screening level estimates of environmental concentration and associated human/ecological exposures.
3 Areas of assessment		*Please check the appropriate box:* Human health (X) Environment (X)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (X) Consumer product exposure (X) Worker exposure ( ) Not Applicable ( ) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (X) Ingestion (X) Dermal (X) Multi-media ( ) Not Applicable ( ) Others. ( ) Comments:
5 Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (X) Marine organisms (X) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others. ( ) Comments.

	(b) Pathways of exposure covered	*Please check the appropriate box* Air ( ) Water (X) Sediment ( ) Soil ( ) Biota ( ) Sewage treatment plant ( ) Multi-media ( ) Not Applicable ( ) Others. ( ) Comments:
6. Type of Information Provided		*Please check the appropriate box* Daily intake (X) Potential dose (X) Margin of safety ( ) Predicted environmental concentration (X) Risk quotient (predicted environmental concentration / predicted no-effect concentration) (X) Others: ( ) Comments. Environmental concentrations and effect levels are compared in the Probabilistic Dilution Model (PDM), which is a component of E-FAST
7. Model Approach		omments E-FAST is a multi-pathway exposure assessment tool designed to provide a screening level assessment. E-FAST is intended to be conservative and the model predictions are likely to be higher than average, as compared to concentrations and exposures that might actually be occurring in a real world setting.
1. Limitations of Model		- The screening level approach is not appropriate for all situations - Data evaluation is critical (garbage in - garbage out). - The various pathways modelled in E-FAST have differing levels of complexity. - Different levels of confidence exist for each of the various exposure pathways. - The preset consumer exposure scenarios are limited to the type of chemicals typically reviewed in the US EPA new chemicals program.
2. Are limitations clearly described for user of Model?		Yes.
3. Which types of chemicals can appropriately be evaluated by the Model?		Both inorganic and organic chemicals
4 Which types of chemicals can NOT be evaluated by the Model?		
1. In what written language is Model available?		English

2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		
3. Does the Model contain a searchable Database?		Yes
4. Is the Model Computerized?		Yes
1. Output / Information provided by the Model		- Environmental concentration in surface water, ambient air, indoor air and groundwater. - Potential human exposures (LADD, ADD and APR) via inhalation, ingestion and dermal contact - The number of days per year an Aquatic Concentration of Concern is exceeded
2. Input data needed to use the Model		- Release amounts from manufacturing, processing, commercial use, industrial use, or the use of consumer products. - Certain relevant p/chem and fate properties - Information on the location of the release activity.
3. (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s).	
	Is the User's Manual incorporated into help screens within the computer model?	Yes
4. Computer hardware requirements		Processor - 486 computer, Memory 16 MB, Hard disk space 48 MB, Operating system: Windows 95, 98, NT, Screen resolution SVGA: 800 x 600.
5. Computer software requirements		
6. Skill / Expertise / Training required to use the Model		Although the model is fairly easy to use, some knowledge of chemistry, as well as exposure and risk assessment may be required to properly interpret the results
1. Has the Model been evaluated with data?		No
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		No
3. Has the Model been published or peer reviewed? If so, provide citation(s)		The Consumer Exposure Pathway of E-FAST has been peer reviewed.
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		
1. Is the Model publicly available, or is it proprietary?		Publically available.

	If it can be downloaded from the Internet, what is the web address (URL)?	www.epa.gov/oppt/exposure
2. How frequently is it updated?		As needed
3. How much does it cost to obtain the Model (if any)?		It is free.
1. Creator, Author or Sponsoring Organization		US Environmental Protection Agency, Office of Pollution Prevention and Toxics.
2. Country of Origin		United States
3. Latest Version number and date of latest update / revision		Beta-version 1.0, May 2000
4. Identify previous versions or contributing elements (names and dates) of the Model		first version
1. Name		Conrad Flessner
2. Affiliation		US EPA
3. Department		Office of Pollution Prevention and Toxics
4. Address		1200 Pennsylvania Avenue, NW (7406M)
5. Postal / Zip code		20460
6. City and Country		Washington, DC
7 Tel / Fax / Email		Tel: 202-564-8541 Email: flessner.conrad@epa.gov

Equilibrium Criterion (EQC) Model

QUESTION		ANSWER
1 What is the Model Name or Unique identifier?		EQC (Equilibrium Criterion Model)
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box:* Regulatory ( ) Research (X) Others. ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	Has been adapted for use in the US EPA's Waste Minimization Prioritization Tool (WIMPT)
3. Areas of assessment		*Please check the appropriate box* Human health ( ) Environment (X)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment ( ) Consumer product exposure ( ) Worker exposure ( ) Not Applicable (X) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation ( ) Ingestion ( ) Dermal ( ) Multi-media ( ) Not Applicable (X) Others: ( ) Comments.
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (X) Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others: ( ) Comments·

	(b) Pathways of exposure covered	*Please check the appropriate box* Air (X) Water (X) Sediment (X) Soil (X) Biota (X) Sewage treatment plant ( ) Multi-media (X) Not Applicable ( ) Others: ( ) Comments:
6. Type of Information Provided		*Please check the appropriate box* Daily intake ( ) Potential dose ( ) Margin of safety ( ) Predicted environmental concentration (X) Risk quotient (predicted environmental concentration / predicted no-effect concentration) ( ) Others: (X) Comments: Regional average concentrations are calculated for an illustrative environment. Bioconcentration Factor is also calculated
7. Model Approach		Comments Deterministic or Probabilistic
1. Limitations of Model		Not designed for site-specific assessments Applicable only to organics and non-speciating metals Evaluation exercises have focused on non-ionising organic chemicals
2. Are limitations clearly described for user of Model?		Appropriate use and limitations are discussed in the series of papers by Mackay et al. (1996 a,b,c).
3. Which types of chemicals can appropriately be evaluated by the Model?		non ionisable organics and non-speciating metals
4. Which types of chemicals can NOT be evaluated by the Model?		speciating metals (eg: mercury)
1. In what written language is Model available?		English
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		No (N/A)
3. Does the Model contain a searchable Database?		Yes, of chemicals with physico-chemical properties, and of regional environmental parameters.
4. Is the Model Computerized?		Yes – Windows Application.
1. Output / Information provided by the Model		Outputs. - media-specific concentrations - regional persistence - advective vs reactive removal of chemical

2. Input data needed to use the Model		(Max. 100 words) Inputs. - physico-chemical properties of the chemical - environment characteristics - estimated emissions
3 (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s)	Shown at time of download http://www.trentu ca/envmodel/
	Is the User's Manual incorporated into help screens within the computer model?	No
4. Computer hardware requirements		Any Windows PC or Power Mac.
5. Computer software requirements		Microsoft Windows 3 1 or 95-98
6. Skill / Expertise / Training required to use the Model		None
1. Has the Model been evaluated with data?		No.
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		Partially validated… Model has been shown to be a useful descriptor of chemical fate over a limited range of its possible applications.
3. Has the Model been published or peer reviewed? If so, provide citation(s)		Yes Mackay (1996 a,b,c)
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		
1. Is the Model publicly available, or is it proprietary?		Publicly available
	If it can be downloaded from the Internet, what is the web address (URL)?	Yes… http://www.trentu.ca/envmodel
2. How frequently is it updated?		Model revisions every 2-3 years.
3. How much does it cost to obtain the Model (if any)?		Free.
1. Creator, Author or Sponsoring Organization		D. Mackay, A. Di Guardo, S. Paterson, C. Cowan.
2. Country of Origin		Canada
3. Latest Version number and date of latest update / revision		Version 1.02 November, 1997.

4. Identify previous versions or contributing elements (names and dates) of the Model	
1. Name	Matthew MacLeod
2. Affiliation	Trent University
3. Department	Canadian Environmental Modelling Centre
4. Address	1600 Westbank Drive
5. Postal / Zip code	K9L 1Y7
6. City and Country	Peterborough, Ontario, Canada
7. Tel / Fax / Email	(705) 748-1011 X 5341 mmacleod@trentu.ca

Full Citations

Mackay D, Paterson, S., Kicsi, G., Di Guardo, A., Cowan, C.E. 1996a. Assessing the Fate of New and Existing Chemicals: A Five Stage Process. Environ. Toxicol. Chem. 15: 1618-1626.

Mackay D, Paterson, S., Di Guardo, A., Cowan, C.E. 1996b. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol. Chem. 15: 1627-1637.

Mackay D, Paterson, S., Kicsi, G., Cowan, C.E., Di Guardo, A., Kane, D.M. 1996c. Assessment of Chemical Fate in the Environment Using Evaluative, Regional and Local-Scale Models: Illustrative Application to Chlorobenzene and Linear Alkylbenzene Sulfonates. Environ. Toxicol. Chem. 15: 1638-1648.

EUSES 1.0

1. Method / Model Name, or Unique identifier		EUSES 1.0
2. Areas of assessment		Human health, Environment
3. Purpose of Method / Model		Regulatory
4. Human health	4.1 Exposure covered	Indirect human exposure via the environment, Consumer product exposure, Worker exposure
	4.2 Routes of exposure covered	Inhalation, Ingestion, Dermal , Multi-media
5. Environment	5.1 Organisms covered	Fresh water organisms, Marine water organisms, Sediment organisms, Terrestrial organisms, Micro-organisms in sewage treatment plant, Fish-and-worm eating predators
	.2 Pathways of exposure covered	Air, Water, Soil, Biota, Sewage treatment plant, Multi-media
6. Type of Information Provided		Daily intake, Potential Dose, Margin of safety, Predicted environmental concentration, Risk Quotient (Predicted environmental concentration / Predicted no-effect concentration), Others
7. Method / Model Approach		Multimedia transport and a transformation model that uses equations based on conservation of mass and chemical equilibrium at three nested spatial scales (continental, regioral and local)
1. Limitations of Method / Model		Chemical risk policy as laid down by the EC (Technical Guidance Documents) A model is always a "cartoon of reality" Expertise of user is important· data evaluation (garbage in, garbage out), interpretation of results Not specifically designed for site-specific substances Model analyses (incl. validation) has been performed to a limited extent Certain process formulations are based on limited research and need to be improved The model results can be unreliable when expertise is lackirg The risk resulting from use of pesticides and biocides are not considered
2. Are Limitations Clearly Described for User of Method?		Yes, specific chapter in manual.
3. Scope of Use of Method / Model - How is Method / Model applied or used?		For the assessment of New and Existing chemicals (according to EU TGDs) Computerised model by diverse assessment modes via a used friendly interface
4. Which types of chemicals can appropriately be evaluated by the method?		Organic chemicals (non-ionic)
5. Which types of chemicals can NOT be evaluated by the method?		Inorganic chemicals, Metals (partly), (fully) dissociating chemicals, Ionic chemicals
1. In what written language is Method / Model available?		English
2. Does Method / Model exists only as an		No

algorithm, and not yet computerised? If so, is algorithm available to User of the Method?	
3. Does Method / Model contains a searchable Database?	No
4. Computerised?	Yes
1 Output / Information provided by Method / Model	Yes, as EUSES (export) file , Ascii file or print-out
2. Input data needed to use Method / Model	"Base set" input is required, according to Annex VIIA of Directive 67/548/EEC (New substances) and Regulation 793/93 (Existing substances). The RA method requires many more parameters to be specified (e.g. partition coeff. and bioconcentration factors). Estimation methods are available The data requirement may vary for different types of substances.
3 Are References or User's Manual provided for User? If so, provide citation(s). Is the "User's Manual" is incorporated into help screens within the computer model?	Yes, extensive user manual (see E 3)
4. Computer hardware requirements	Minimal: 80386 DX processor (25 MHz), 4 Mb RAM, VGA display, Fixed drive with 10 Mb available, mouse. Recommended: 80486 DX or Pentium processor (>50MHz) and >8 Mb RAM
5 Computer software requirements	Minimal: Windows 3.1
6. Skill / Expertise / Training required to use Method / Model	Expertise is required. EUSES is designed for skilled risk managers in government agencies, scientific institutes and industry.
1. Has Method / Model been evaluated with data?	Only to a limited extent
2 Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?	Partial validation by RIVM and University of Osnabrück, since validation of the risk estimates (PEC/PNEC, Margin of Safety) for the standard scenario over the whole RA chain is not possible. Algorithm validation and software evaluation have been performed. Numerical validation activities for parts of EUSES (modules or submodels) have been performed by comparison with measured data for several chemicals from different chemical classes. A qualitative validation has been performed against expert opinions. Uncertainty analysis and sensitivity analysis have also been performed Explicit criteria have not been formulated by risk assessors or risk managers.
3 Has Method / Model been Published or peer reviewed? If so, provide citation(s).	EC (1996) EUSES, The European Union System for the Evaluation of Substances. National Institute of Public Health and the Environment (RIVM), the Netherlands. Available from the European Chemicals Bureau (EC/JRC), Ispra, Italy. Vermeire, T.G. et al. (1997) European Union System for the Evaluation of Substances (EUSES) Principles and Structure. Chemosphere 34: 1823-1836.
4. Have Method / Model evaluation or validation study(ies) been Published or Peer reviewed? If so, provide citation(s)	Jager, T. (1998) Evaluation of EUSES: inventory of experiences and validation activities. Bithoven, RIVM, Report no. 679102048. Available through RIVM (www rivm.nl) Jager, T. et al. (2000) Probabilistic risk assessment for new and

	existing chemicals: sample calculations. Bilthoven, RIVM, Report no. 679102049. Available through RIVM (www.rivm.nl) Berding, B. et al.. (1999) Visualisation of the complexity of EUSES. Environ. Sci. Pollut.Res. 6: 37-43. Schwartz , S. et al (1998) Quality criteria for environmental risk software – Using the example of EUSES Environ Sci. Pollut.Res 5: 217-222 Shwartz, S., Trapp, S. and Matthies, M. (1997) Preliminary statement on EUSES R&D-project FKZ 106 01 075 of the Federal Environmental Agency, Berlin Validation of environmental exposure models and their parameters.
1. Is Method / Model Publicly Available, or is it Proprietary? If it can be downloaded from the internet, what is the web address?	Yes, publicly available
2. What is frequency of updates?	Planned: Every 4-5 years, together with the update of Technical Guidance Document
3. What is Cost of obtaining Method / Model (if any)	180 Euro
1. Creator, Author or Sponsoring Organisation	EUSES has been prepared by the National Institute of Public Health and the Environment (RIVM)
2. Country of Origin	The Netherlands (together with EU member states)
3. Latest Version number and Date of latest update / revision	Version 1.0 December 1996
4 Identify previous versions or contributing elements (names and dates) of method	USES 1.0 (1994) and EU-TGD New and Existing substances (1996)
H. CONTACT PERSON	
1. Name	Christian Heidorn
2. Affiliation	European Chemicals Bureau
3 Department	JRC Environment Institute
4. Address	
5. Postal / Zip code	I-21020
6 City and Country	Ispra (Varese) Italy
7. Tel / Fax / Email	Tel: + 39 0332 785866 Fax: + 39 0332 785862 e-mail: euses.euses@jrc.it

Geographical Exposure Modeling System (GEMS)

QUESTION		ANSWER
1 What is the Model Name or Unique identifier?		Geographical Exposure Modeling System (GEMS)
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box.* Regulatory (X) Research ( ) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	The United States Environmental Protection Agency and many others in government, academia, and industry used earlier versions of GEMS and PCGEMS to model environmental concentrations of new and existing chemicals. The predicted environmental concentrations were used to prepare exposure assessments and risk assessments to support decision-making by risk managers The new version of GEMS will have similar uses.
3 Areas of assessment		*Please check the appropriate box* Human health (X) Environment (X)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (X) Consumer product exposure ( ) Worker exposure ( ) Not Applicable ( ) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (X) Ingestion (X) Dermal (X) Multi-media (X) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (X) Marine organisms ( ) Sediment organisms (X) Terrestrial organisms (X) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others. ( )

		Comments:
	(b) Pathways of exposure covered	*Please check the appropriate box* Air (X) Water (X) Sediment (X) Soil (X) Biota ( ) Sewage treatment plant ( ) Multi-media (X) Not Applicable ( ) Others: ( ) Comments.
6. Type of Information Provided		*Please check the appropriate box* Daily intake ( ) Potential dose (X) Margin of safety ( ) Predicted environmental concentration (X) Risk quotient (predicted environmental concentration / predicted no-effect concentration) ( ) Others. ( ) Comments:
7. Model Approach		CommentsGEMS will bring together in one system several U.S. EPA environmental fate and transport models for ambient air, surface water, soil, and ground water, and some of the data needed to run the models. GEMS will make the models easier to use than their stand-alone counterparts GEMS will have interactive menus to guide the user in selecting models, selecting and organizing data to be used as input to model runs, executing model runs, and presenting model outputs. The menus will also provide user help
1. Limitations of Model		GEMS is under development and is not yet available.
2. Are limitations clearly described for user of Model?		GEMS is under development.
3 Which types of chemicals can appropriately be evaluated by the Model?		Organic chemicals, metals and other inorganic chemicals.
4. Which types of chemicals can NOT be evaluated by the Model?		Unknown.
1. In what written language iis Model available?		English.
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		GEMS is under development and is not yet available.
3. Does the Model contain a searchable Database?		Yes, when GEMS is complete.
4. Is the Model Computerized?		GEMS is under development.

1. Output / Information provided by the Model		GEMS will have statistical analysis, graphics, and Geographical Information System (GIS) capabilities for analyzing and displaying data and environmental modelling results.
2. Input data needed to use the Model		The input data needed are different for each model in GEMS The input data generally include physical-chemical properties and site-specific information, such as site location, emission estimates, stack parameters, etc.
3. (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s)	User's manuals will be included in the on-line user help.
	Is the User's Manual incorporated into help screens within the computer model?	Yes, when GEMS is complete.
4. Computer hardware requirements		Full hardware requirements are to be determined. A personal computer with a modem will be required
5. Computer software requirements		Full software requirements are to be determined A web browser such as Netscape or Internet Explorer will be required
6 Skill / Expertise / Training required to use the Model		Requires some knowledge of environmental science and some skill in the use of computers.
1. Has the Model been evaluated with data?		GEMS has not been evaluated with data. Some of the models in GEMS have been evaluated with data.
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		GEMS has not been validated. Some of the models in GEMS have been validated.
3. Has the Model been published or peer reviewed? If so, provide citation(s).		The new version of GEMS is under development and has not been published or peer reviewed Some of the models in GEMS have been published or peer reviewed
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		Unknown.
1. Is the Model publicly available, or is it proprietary?		GEMS is under development and is not yet available. GEMS will be publicly available to anyone through the Internet by March, 2001. GEMS will not be proprietary.
	If it can be downloaded from the Internet, what is the web address (URL)?	The new GEMS will be publicly available to anyone through the Internet by March, 2001. The URL is to be determined.
2. How frequently is it updated?		To be determined.
3. How much does it cost to obtain the Model (if any)?		No cost other than hardware and software costs.
1. Creator, Author or Sponsoring Organization		United States Environmental Protection Agency
2. Country of Origin		United States

3. Latest Version number and date of latest update / revision	To be determined.
. Identify previous versions or contributing elements (names and dates) of the Model	GEMS (Graphical Exposure Modeling System) PCGEMS (Personal Computer version of Graphical Exposure Modeling System) TRIAIR (Toxic Release Inventory Air model) ISCLT (Industrial Source Complex Long Term model) ISCST (Industrial Source Complex Short Term model) TRIWATER (Toxic Release Inventory Water model) PROUTE (Pollutant Routing model) EXAMS (Exposure Analysis Modeling System model) SESOIL (Seasonal Soil model) AT123D (Analytical Transient 1-, 2-, or 3-Dimensional simulation of waste transport model) Dates: early 1980s to present
1 Name	Ms Lynn Delpire
2. Affiliation	United States Environmental Protection Agency
3. Department	Office of Prevention, Pesticides and Toxic Substances Office of Pollution Prevention and Toxics Economics, Exposure and Technology Division Exposure Assessment Branch
4. Address	1200 Pennsylvania Ave., N.W. (7406)
5 Postal / Zip code	20460
6. City and Country	Washington, DC, USA
7. Tel / Fax / Email	Tel: 202-260-3928 Fax· 202-260-0981 e-mail: delpire.lynn@epa.gov

PROAST Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		PROAST
2 Purpose / Use of Model	(a) Purpose	*Please check the appropriate box:* Regulatory (x) Research (x) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	RIVM TNO IRAS (University of Utrecht)
3. Areas of assessment		*Please check the appropriate box.* Human health (x) Environment ()
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (x) Consumer product exposure (x) Worker exposure (x) Not Applicable ( ) Others: any human exposure (x) Comments.
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (x) Ingestion (x) Dermal (x) Multi-media (x) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms ( ) Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable ( ) Others. any organism ( ) Comments:
	(b) Pathways of exposure covered	*Please check the appropriate box* Air ( )

		Water	( )
		Sediment	( )
		Soil	( )
		Biota	( )
		Sewage treatment plant	( )
		Multi-media	( )
		Not Applicable	( )
		Others	( )
		Comments:	
6. Type of Information Provided		*Please check the appropriate box*	
		Daily intake	( )
		Potential dose	( )
		Margin of safety	( )
		Predicted environmental concentration	( )
		Risk quotient (predicted environmental concentration / predicted no-effect concentration)	( )
		Others: RfD or possible human health effects, both with uncertainty margins	( )
		Comments:	
7 Model Approach		Comments fit dose-response model to dose-response data, then apply probabilistic assessment factors, resulting in uncertainty distribution for exposure limit or, uncertainty distribution for specific health effect in sensitive human being, given a particular exposure level	
1. Limitations of Model		- dose-response data needed with several response levels	
2. Are limitations clearly described for user of Model?		not yet	
3. Which types of chemicals can appropriately be evaluated by the Model?		all, if dose-response data available	
4 Which types of chemicals can NOT be evaluated by the Model?		none	
1. In what written language is Model available?		English	
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		no	
3. Does the Model contain a searchable Database?		no	
4 Is the Model Computerized?		yes	
1. Output / Information provided by the Model		- fitted dose-response model - Critical Effect Dose (CED) with confidence interval - uncertainty distribution for CED in sensitive human - uncertainty distribution for possible health effect in sensitive human	
2. Input data needed to use the Model		dose-response data	
3 (a) Are References or User's Manual provided for User?		Yes (in Dutch, English in prep)	(x)
		No	( )

(b) If YES	Provide citation(s)	
	Is the User's Manual incorporated into help screens within the computer model?	
4. Computer hardware requirements		PC
5. Computer software requirements		Splus
6. Skill / Expertise / Training required to use the Model		Basic statistics
1. Has the Model been evaluated with data?		yes
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		yes, it has been applied to many different data sets from studies in diverse fields in toxicology.
3 Has the Model been published or peer reviewed? If so, provide citation(s).		yes: - Slob W. and M.N.Pieters (1998). Risk Analysis 18: 787-798. - Vermeire T, Stevenson H, Pieters MN, Rennen M, Slob W, Hakkert BC (1999) Crit. Rev. Toxicol 29: 439-490 - W. Slob (1999). In: Statistics for the Environment 4. Statistical Aspects of Health and the Environment (V. Barnett, A. Stein, KF Turkman, eds): 153-174
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		yes, AH Piersma, A Verhoef, JD te Biesebeek, MN Pieters, W Slob (2000). Developmental and testicular toxicity of butyl benzyl phthalate in the rat using a multiple dose study design. (in press)
1. Is the Model publicly available, or is it proprietary?		proprietary, but will be made publicly available
	If it can be downloaded from the Internet, what is the web address (URL)?	
2. How frequently is it updated?		several times a year
3. How much does it cost to obtain the Model (if any)?		
1. Creator, Author or Sponsoring Organization		W. Slob, RIVM
2. Country of Origin		The Netherlands
3 Latest Version number and date of latest update / revision		PROAST.V70
4. Identify previous versions or contributing elements (names and dates) of the Model		
1. Name		Prof.dr Wout Slob
2. Affiliation		RIVM

3. Department	LEO
4. Address	PO BOX 1
5. Postal / Zip code	3720 BA
6. City and Country	Bilthoven, The Netherlands
7. Tel / Fax / Email	tel· 31 30 2743242 fax: 31 30 274 4446 e-mail: wout.slob@rivm nl

Use Cluster Scoring System (UCSS) Model

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		Use Cluster Scoring System (UCSS)
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box* Regulatory (X) Research ( ) Others: Priority Setting (X)
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	EPA, chemical industries, EPA regions, OSHA. a number of state governments have used this system to set priorities for their regulatory and non-regulatory pollution prevention and risk reduction efforts.
3 Areas of assessment		*Please check the appropriate box* Human health (X) Environment (X)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (X) Consumer product exposure ( ) Worker exposure (X) Not Applicable ( ) Others ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (X) Ingestion (X) Dermal (X) Multi-media (X) Not Applicable ( ) Others: ( ) Comments:
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms () Marine organisms ( ) Sediment organisms ( ) Terrestrial organisms ( ) Micro-organisms in sewage treatment plant ( ) Fish-and-worm eating predators ( ) Not Applicable (X) Others: ( ) Comments:
	(b) Pathways of	*Please check the appropriate box*

	exposure covered	Air (X) Water (X) Sediment (X) Soil (X) Biota ( ) Sewage treatment plant ( ) Multi-media (X) Not Applicable ( ) Others. ( ) Comments:
6. Type of Information Provided		*Please check the appropriate box* Daily intake ( ) Potential dose ( ) Margin of safety ( ) Predicted environmental concentration ( ) Risk quotient (predicted environmental concentration / predicted no-effect concentration) ( ) Others (X) Comments:
7. Model Approach		Comments This is a computerized priority setting tool for the existing chemicals used in industrial and/or commercial settings. Under UCSS, chemicals are grouped based on their uses and are ranked based on their hazard and exposure.
1. Limitations of Model		The exposure information used in the model is just a surrogate for the actual exposure and therefore the actual exposure may be significantly different from that predicted by the system. Only a very limited industrial and commercial uses for the TSCA chemicals are captured in the system. Only those chemicals with a complete set of information on both hazard and exposure are included and leaves out many chemicals with partial data.
2. Are limitations clearly described for user of Model?		yes, they are included in the users manual.
3. Which types of chemicals can appropriately be evaluated by the Model?		TSCA chemicals used in industrial and commercial settings.
4. Which types of chemicals can NOT be evaluated by the Model?		Does not include non-TSCA chemicals, and TSCA chemicals without adequate toxicity and exposure data.
1. In what written language is Model available?		English
2. Does the Model exist only as an algorithm, and not yet computerized? If so, is algorithm available to User?		The model exists as a working computerized system. In addition, the algorithm for the system is clearly described in the document.
3. Does the Model contain a searchable Database?		yes
4. Is the Model Computerized?		yes

1. Output / Information provided by the Model		Scores for the clusters Human exposure, Ecological exposure, Human toxicity and ecological toxicity scores for the chemicals
2. Input data needed to use the Model		Use of the chemical. Exposure information of the chemical (use volume, number of workers, site, release to the environment) Persistence and Bioaccumulation information. Both ecological and human toxicity information.
3. (a) Are References or User's Manual provided for User?		Yes (X) No ( )
(b) If YES	Provide citation(s).	
	Is the User's Manual incorporated into help screens within the computer model?	NO
4. Computer hardware requirements		a desktop personal computer with minimum of Pentium II processor with 32 meg of ram and 15 meg of hard drive space for the system
5 Computer software requirements		Windows based operating system, (Windows 95 or above)
6. Skill / Expertise / Training required to use the Model		Basic understanding of chemical risk assessment and some understanding of industrial chemical uses Basic understanding of Window 95.
1. Has the Model been evaluated with data?		Not applicable
2. Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		Both the computerized system and the underlying methodologies have under gone an EPA Science Advisory Board review.
3. Has the Model been published or peer reviewed? If so, provide citation(s).		see above
4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s).		see above
1. Is the Model publicly available, or is it proprietary?		Yes they are available to public.
	If it can be downloaded from the Internet, what is the web address (URL)?	Not at this point
2 How frequently is it updated?		once a year
3. How much does it cost to obtain the Model (if any)?		none
1. Creator, Author or Sponsoring Organization		U.S. EPA

2. Country of Origin	USA
3. Latest Version number and date of latest update / revision	1998
4. Identify previous versions or contributing elements (names and dates) of the Model	
1. Name	Jay Jon
2 Affiliation	
3. Department	U.S. Environmental Protection Agency
4 Address	1200 Pennsylvania Avenue NW
5. Postal / Zip code	20460
6 City and Country	United States of America
7 Tel / Fax / Email	202-260-7971 / 202-260-0816

USES 3.0

QUESTION		ANSWER
1. What is the Model Name or Unique identifier?		USES 3 0
2. Purpose / Use of Model	(a) Purpose	*Please check the appropriate box:* Regulatory (x) Research ( ) Others: ( )
	(b) What government(s) and/or government organization(s) have used or are using the Model and in what application or capacity?	Risk assessors in government and industry in The Netherlands and many other countries inside and outside the EU. Purpose Risk assessment of new and existing substances (equivalent to EUSES 1.00) and of agricultural pesticides and biocides.
3. Areas of assessment		*Please check the appropriate box:* Human health (x) Environment (x)
4. Human health	(a) Exposure covered	*Please check the appropriate box* Indirect human exposure via the environment (x) Consumer product exposure (x) Worker exposure (x) Not Applicable ( ) Others: ( ) Comments:
	(b) Routes of exposure covered	*Please check the appropriate box* Inhalation (x) Ingestion (x) Dermal (x) Multi-media (x) Not Applicable ( ) Others: ( ) Comments.
5. Environment	(a) Organisms covered	*Please check the appropriate box* Freshwater organisms (x) Marine organisms (x) Sediment organisms (x) Terrestrial organisms (x) Micro-organisms in sewage treatment plant (x) Fish-and-worm eating predators (x) Not Applicable ( ) Others: ( ) Comments.
	(b) Pathways of exposure covered	*Please check the appropriate box* Air (x) Water (x) Sediment (x)

		Soil	(x)
		Biota	(x)
		Sewage treatment plant	(x)
		Multi-media	(x)
		Not Applicable	( )
		Others	( )
		Comments.	
6. Type of Information Provided		*Please check the appropriate box*	
		Daily intake	(x)
		Potential dose	(x)
		Margin of safety	(x)
		Predicted environmental concentration	(x)
		Risk quotient (predicted environmental concentration / predicted no-effect concentration)	(x)
		Others.	( )
		Comments:	
7. Model Approach		Multimedia transport and a transformation model that uses equations based on conservation of mass and chemical equilibrium at three nested spatial scales (continental, regional and local)	
1. Limitations of Model		Chemical risk policy as laid down by the EC (Technical Guidance Documents) A model is always a "cartoon of reality" Expertise of user is important: data evaluation (garbage in, garbage out), interpretation of results Not specifically designed for site-specific assessments Model analyses (incl validation) has been performed to a limited extent Certain process formulations are based on limited research and need to be improved The model results can be unreliable when expertise is lacking	
2. Are limitations clearly described for user of Model?		Yes, specific chapter in manual	
3. Which types of chemicals can appropriately be evaluated by the Model?		Organic chemicals (non-ionic), metals (with some adaptations)	
4 Which types of chemicals can NOT be evaluated by the Model?		Inorganic chemicals, metals (partly), (fully) dissociating chemicals, ionic chemicals	
1. In what written language is Model available?		English	
2. Does the Model exist only as an algorithm, and not yet computerised? If so, is algorithm available to User?		No	
3. Does the Model contain a searchable Database?		No. A searchable database is built while using the model.	
4. Is the Model Computerized?		Yes	
1. Output / Information provided by the Model		EUSES (export) file , Ascii file or print-out	

2. Input data needed to use the Model		"Base set" input is required, according to Annex VIIA of Directive 67/548/EEC (New substances) and Regulation 793/93 (Existing substances) or in line with the pesticide admission requirements. The RA method requires many more parameters to be specified (e.g. emission factors, partition coeff. and bioconcentration factors). Estimation methods are available. The data requirement may vary for different types of substances.
3. (a) Are References or User's Manual provided for User?		Yes, extensive technical + user manual (x)
(b) If YES	Provide citation(s)	RIVM, VROM, VWS (1999) Uniform System for the Evaluation of Substances 3.0 (USES 3.0) Natonal Institute of Public Health and the Environment (RIVM). Ministry of Housing, Spatial Planning and the Environment (VROM, Ministry of Health, Welfare and Sport (VWS) The Netherlands. RIVM report 601450 004.
	Is the User's Manual incorporated into help screens within the computer model?	Yes
4. Computer hardware requirements		Minimal: 80386 DX processor (25 MHz), 4 Mb RAM, VGA display, Fixed drive with 10 Mb available, mouse. Recommended: 80486 DX or Pentium processor (>50MHz) and >8 Mb RAM
5. Computer software requirements		Minimal: Windows 3.1
6. Skill / Expertise / Training required to use the Model		Expertise is required. USES is designed for skilled risk managers in government agencies, scientific institutes and industry
1. Has the Model been evaluated with data?		Only to a limited extent
2 Do you consider the model to have been validated? If so, what was the validation method(s) and criteria? Has the model been validated over the full range of its possible application or over a more limited range?		Partial validation of the EUSES part by RIVM and University of Osnabrück, since validation of the risk estimates (PEC/PNEC, Margin of Safety) for the standard scenario over the whole RA chain is not possible. Algorithm validation and software evaluation have been performed. Numerical validation activities for parts of EUSES (modules or submodels) have been performed by comparison with measured data for several chemicals from different chemical classes. A qualitative validation has been performed against expert opinions Uncertainty analysis and sensitivity analysis have also been performed. The validation status of the pesticides part is low. Explicit criteria have not been formulated by risk assessors or risk managers.
3. Has the Model been published or peer reviewed? If so, provide citation(s).		RIVM, VROM, VWS (1999) Uniform System for the Evaluation of Substances 3.0 (USES 3.0). Natonal Institute of Public Health and the Environment (RIVM). Ministry of Housing, Spatial Planning and the Environment (VROM, Ministry of Health, Welfare and Sport (VWS). The Netherlands. RIVM report 601450 004. Vermeire, T G. et al. (1997) European Union System for the Evaluation of Substances (EUSES) Principles and Structure. Chemosphere 34: 1823-1836 Vermeire, T.G. et al. (1994) Uniform System for the Evaluation of Substances I,II,III,IV,V. Publications in Chemosphere, 29:23-38, 319-335, 337-352, 353-369 and Chemosphere 31. 3237-3248, respectively.

4. Have the Model evaluation or validation study(ies) been published or peer reviewed? If so, provide citation(s)		(Max 100 words)
1. Is the Model publicly available, or is it proprietary?		(Max. 100 words)
	If it can be downloaded from the Internet, what is the web address (URL)?	
2 How frequently is it updated?		(Max. 100 words)
3. How much does it cost to obtain the Model (if any)?		(Max. 100 words)
1. Creator, Author or Sponsoring Organization		
2. Country of Origin		
3 Latest Version number and date of latest update / revision		
4. Identify previous versions or contributing elements (names and dates) of the Model		
1. Name		
2 Affiliation		
3. Department		
4. Address		
5. Postal / Zip code		
6. City and Country		
7. Tel / Fax / Email		